Kathleen Fuller or Mary Hall, please!

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

7-226

Requestor's Name: OSWECKI, JANE - RM 3E15 Serial Number: 08/925,326

Date: 7/7/98 Phone: 305-7152 Art Unit: 1613

Search Topic:
Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

Please search N-substituted indol-3-glyoxylamides of claim 1 for general formulae, claim 2 for specific compounds, and claim 8 for two separate processes for preparing these compounds. Claims 1, 2 and 8 are highlighted appropriately and attached.*

Inventors: Guillaume Lebault
Cecillia Menciu
Bernhard Kutscher
Peter Emig
Stefan Szelenyi
and
Kay Brune

1998 JUL -9 AM 8:42

Thank you!

* Please use non-highlighted information to whatever extent it is helpful in your search, but otherwise please simply ignore it.

78

STAFF USE ONLY

Date completed: 7/15/98 308-4290
Searcher: K. Fuller RM
Terminal time: 60 1E01
Elapsed time:
CPU time:
Total time: 95
Number of Searches: 1
Number of Databases:
subset

Search Site
- ___ STIC
- ✓ CM-1
- ___ Pre-S

Type of Search
- ___ N.A. Sequence
- ___ A.A. Sequence
- ✓ Structure
- ___ Bibliographic

Vendors
- ___ IG
- ✓ STN
- ___ Dialog
- ___ APS
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- ___ SDC
- ___ DARC/Questel
- ___ Other

PTO-1590 (9-90)

=> FILE REG

FILE 'REGISTRY' ENTERED AT 10:44:06 ON 15 JUL 1998
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 10 JUL 98 HIGHEST RN 208329-94-6
DICTIONARY FILE UPDATES: 14 JUL 98 HIGHEST RN 208329-94-6

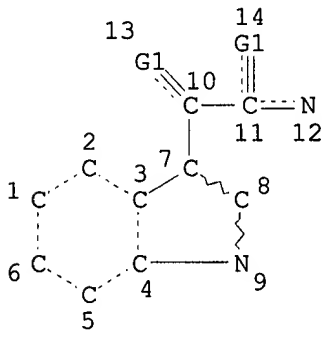
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 14, 1998

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Stereochemical name changes have been adopted and appear in CN's beginning 6/29/30. See the online news message for details.

=> D QUE L22

L4 STR



1460 structures from broad search

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STEREO ATTRIBUTES: NONE
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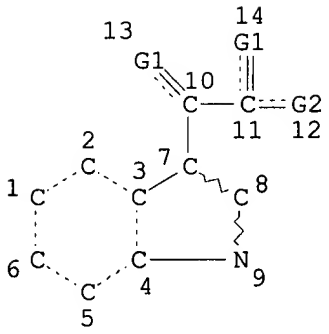

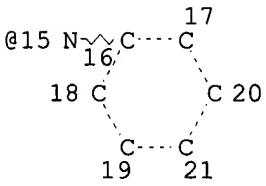

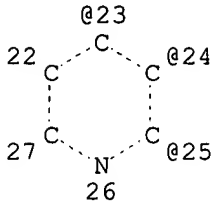

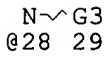

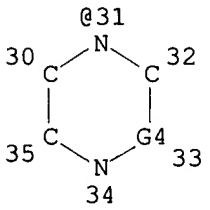

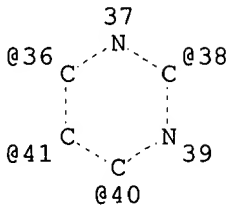

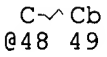

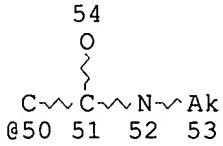

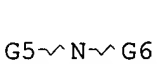

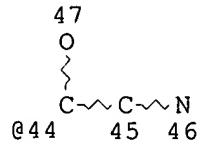

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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE
L22 204 SEA FILE=REGISTRY SUB=L7 SSS FUL L20

=> FILE HCAPLUS

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FILE COVERS 1967 - 15 Jul 1998 VOL 129 ISS 3
FILE LAST UPDATED: 15 Jul 1998 (980715/ED)

This file contains CAS Registry Numbers for easy and accurate

204 structures from subset search of the 1460 structures

substance identification.

This file now supports REGlstRY for direct browsing and searching of all non-structural data from the REGISTRY file. Enter HELP FIRST for more information.

=> D HIS L23-L24

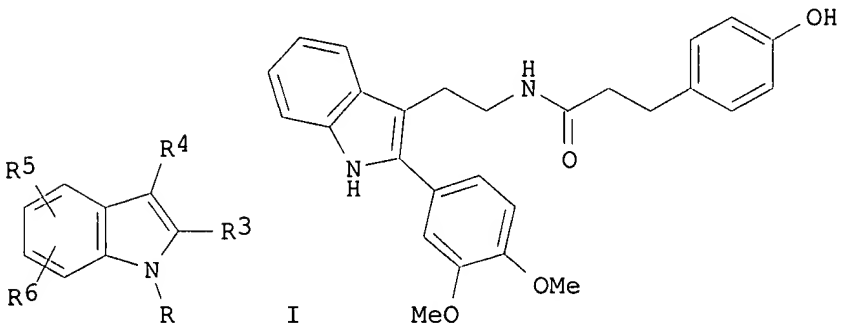
(FILE 'REGISTRY' ENTERED AT 09:32:27 ON 15 JUL 1998)
SAVE L22 OSW925SS/A

FILE 'HCAPLUS' ENTERED AT 10:35:03 ON 15 JUL 1998
L23 33 S L22
L24 30 S L23(L)(PREP OR SPN)/RL

=> D L24 1-30 CBIB ABS IND HITSTR

L24 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1998:394035 Preparation of N-aralkyl-2-(substituted-aryl)indole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists. Goulet, Mark; Chu, Lin; Ashton, Wallace T.; Fisher, Michael H.; Wyvratt, Matthew J.; Smith, Roy G.; Bugianesi, Robert L.; Ponpipom, Mitree M.; Yang, Yi Tien; Lin, Peter (Merck and Co., Inc., USA). U.S. US 5756507 A 980526, 53 pp. (English). CODEN: USXXAM. APPLICATION: US 96-760851 961205.

GI



I II

AB Title compds. I [R = H, (ar)alkyl, aryl, etc.; R4 = (CR9R9a)mCR10R10aNR2ZR1; R1 = (un)substituted Ph, -naphthyl, -biphenylyl, etc.; R2 = H, (ar)alkyl, aryl, etc.; R3 = Ph with 2-3 substituents; R5 = H, halo, OR7, OR8, NR7R8, COR7, COR8, etc.; R6 = H, halo, (perfluoro)alkyl, aryl, etc.; R7 = H or (un)substituted alkyl; R8 = H, CO2H derivs., NH2 or derivs., etc.; R9, R9a = H, (ar)alkyl, aryl, etc.; R10, R10a = H, (ar)alkyl, aryl, etc.; Z = (un)substituted alk(en/yn)ylene, etc.; NR2Z = heterocyclene; m = 0-3] and their pharmaceutically acceptable salts are antagonists of GnRH (gonadotropin releasing hormone), and are useful for the treatment of a variety of sex-hormone-related and other conditions in both men and women (no data). Almost 300 invention compds. were prepd. and/or claimed. For instance, amidation of 3-(4-hydroxyphenyl)propionic acid with 2-[2-(3,4-dimethoxyphenyl)-1H-indol-3-yl]ethylamine using EDC and HOBt gave title compd. II.

IC ICM A61K031-405
ICS A61K031-495; C07D209-10; C07D403-06

NCL 514255000
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 2
ST arylindolealkanamine prepn gonadotropin releasing hormone antagonist
IT Uterine tumors
(myoma, treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Puberty
(precocious puberty, treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Antitumor agents
Contraceptives
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Gonadotropin-releasing hormone receptor
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Growth disorders (animal)
(short stature, treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Apnea
(sleep apnea, treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Breast tumors
Endometriosis
Growth hormone deficiency
Hirsutism
Irritable bowel syndrome
Lupus erythematosus
Pituitary adenoma
Polycystic ovary syndrome
Premenstrual syndrome
Prostatic hyperplasia
Prostatic tumors
Uterine leiomyoma
Uterine tumors
(treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT Myoma
(uterine, treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)
IT 6686-26-6P 15741-71-6P 19571-34-7P 36924-81-9P, Ethyl 2-(4-aminophenyl)-2-methylpropionate 50712-64-6P, Ethyl 2-(4-Nitrophenyl)propionate 53157-45-2P 64214-66-0P 65476-32-6P 79606-42-1P 79606-48-7P 83397-45-9P 137402-61-0P 150668-36-3P 172975-69-8P, 3,5-Dimethylphenylboronic acid 192182-01-7P 192182-34-6P 192182-46-0P 192182-48-2P 192643-78-0P 192643-86-0P 192643-90-6P 192644-20-5P 192644-21-6P 192717-28-5P 192770-58-4P 192770-59-5P 192770-60-8P 192770-62-0P 192770-63-1P 192770-65-3P 192770-66-4P 192770-67-5P 192770-69-7P 192770-70-0P 192770-71-1P 192770-72-2P 192770-73-3P 192770-74-4P 192770-75-5P 192770-76-6P 192770-77-7P 192773-91-4P 192773-92-5P 192773-93-6P 192773-94-7P 192773-95-8P 192773-96-9P 192773-97-0P 192773-98-1P 192773-99-2P 192774-00-8P 192774-01-9P 192774-02-0P 192774-03-1P 192774-04-2P 192774-05-3P 192774-06-4P 192774-07-5P 192774-08-6P 192774-09-7P 192774-10-0P 192774-11-1P

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192774-22-4P 192774-23-5P 192774-24-6P **192774-25-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(intermediate; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

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RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

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RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

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RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

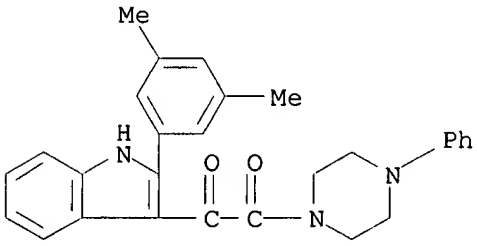
IT 107950-52-7, Gonadotropin-releasing hormone
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 61-54-1, 1H-Indole-3-ethanamine 79-44-7, Dimethylcarbamyl chloride 92-54-6, 1-Phenylpiperazine 100-39-0, Benzyl bromide 104-03-0, 4-Nitrophenylacetic acid 107-10-8, 1-Propanamine 108-18-9, Diisopropylamine 109-89-7, Diethylamine 501-53-1, Benzyl chloroformate 501-97-3, 3-(4-Hydroxyphenyl)propionic acid 556-96-7, 5-Bromo-m-xylene 619-67-0, 4-Hydrazinobenzoic acid 4635-59-0, 4-Chlorobutyryl chloride 5438-70-0, Ethyl 4-aminophenylacetate 5600-62-4, 4-(4-Nitrophenyl)butyric acid 6293-83-0, 2-Iodo-4-nitroaniline 6366-06-9, 3,5-Dimethylphenylacetylene 13436-46-9, 2-Ethoxytetrahydrofuran 19910-33-9, 2-(4-Nitrophenyl)propionic acid 20776-45-8, 5-Benzyloxytryptamine 22205-09-0, 4-(4-Aminobutyl)phenol 22509-74-6, N-Ethoxycarbonylphthalimide 29555-02-0, 2-Methylcyclopropanecarboxylic acid 34674-93-6, 4-(4-Hydroxyphenyl)butyric acid 53672-98-3 95426-76-9 96090-12-9 105640-07-1 192717-25-2 192774-26-8 192774-27-9
RL: RCT (Reactant)
(starting material; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT **192774-25-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(intermediate; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

RN 192774-25-7 HCAPLUS

CN Piperazine, 1-[[2-(3,5-dimethylphenyl)-1H-indol-3-yl]oxoacetyl]-4-phenyl- (9CI) (CA INDEX NAME)



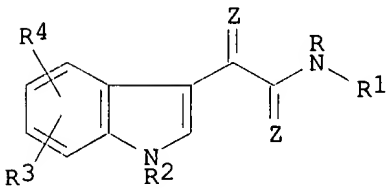
applicant

L24 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 1998 ACS

1998:175908 Document No. 128:217285 Preparation of new, N-substituted indole-3-glyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators. Lebaut, Guillaume; Menciu, Cecilia; Kutscher, Bernhard; Emig, Peter; Szelenyi, Stefan; Brune, Kay (Asta Medica Aktiengesellschaft, Germany). PCT Int. Appl. WO 9809946 A1 980312, 40 pp. DESIGNATED STATES: W: AU, BR, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RU, SG, SK, TR, UA; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 97-EP4474 970816. PRIORITY: DE 96-19636150 960906.

Covers specific compounds in claim 2

GI



I

AB The title compds. [I; R = H, (un)substituted C1-6 alkyl; R1 = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; RR1 = atoms to close (N-substituted) piperazine ring; R2 = H, (un)substituted C1-6 alkyl, (un)substituted benzoyl; R3, R4 = H, OH, C1-6 alkyl, C3-7 cycloalkyl, halo, NO2, amino, benzyloxy, etc.; Z = O, S] and their acid salts were prepd., e.g., by N-alkylation of indoles with R2-bearing reactants followed by acylation with a dicarbonyl halide and amidation of the remaining acid halide function. For example, a title compd. I (R = R3 = R4 = H, R1 = 4-pyridyl, R2 = 4-FC6H4CH2, Z = O) (prepn. by benzylation of indole with 4-FC6H4CH2Cl, acylation of the intermediate with (COCl)2 and amidation of the acyl chloride with 4-aminopyridine given) at 10 mg/kg i.p. in guinea pigs gave 55.4% inhibition of allergen-induced late-phase eosinophilia, vs. 47.0 for cyclosporin A.

IC ICM C07D209-18
ICS C07D401-12; A61K031-40

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

ST indoleglyoxylamide prepn antiasthmatic; antiallergic N pyridyl fluorobenzylindolylglyoxylamide prepn; immunosuppressant indoleglyoxylamide prepn; indole benzylation fluorobenzyl chloride antiasthmatic prepn; oxalyl chloride acylation fluorobenzylindole

antiasthmatic prepn; amidation fluorobenzylindoleglyoxylyl chloride aminopyridine antiasthmatic prepn

IT Allergy inhibitors
Antiasthmatics
Immunosuppressants
(prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT 352-11-4
RL: RCT (Reactant)
(N-benzylation of indole; prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT 120-72-9, Indole, reactions
RL: RCT (Reactant)
(N-benzylation with 4-fluorobenzyl chloride; prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT 79-37-8, Oxalyl chloride
RL: RCT (Reactant)
(acylation of 1-(4-fluorobenzyl)indole; prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT 504-24-5, 4-Aminopyridine
RL: RCT (Reactant)
(amidation of [N-(4-fluorobenzyl)indolyl]glyoxylyl chloride; prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT 204205-77-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation with oxalyl chloride; prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT **152721-57-8P 204205-78-7P 204205-79-8P**
204205-80-1P 204205-81-2P 204205-82-3P
204205-83-4P 204205-84-5P 204205-85-6P
204205-86-7P 204205-87-8P 204205-88-9P
204205-89-0P 204205-90-3P 204205-91-4P
204205-92-5P 204205-93-6P 204205-94-7P
204205-95-8P 204205-96-9P 204205-97-0P
204205-98-1P 204205-99-2P 204206-00-8P
204206-01-9P 204206-02-0P 204206-03-1P
204206-04-2P 204206-05-3P 204206-06-4P
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

IT **152721-57-8P 204205-78-7P 204205-79-8P**
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204205-92-5P 204205-93-6P 204205-94-7P
204205-95-8P 204205-96-9P 204205-97-0P
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204206-01-9P 204206-02-0P 204206-03-1P
204206-04-2P 204206-05-3P 204206-06-4P
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of N-substituted indoleglyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators)

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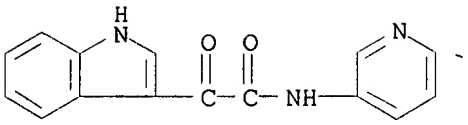
NAME)



RN 204205-78-7 HCAPLUS
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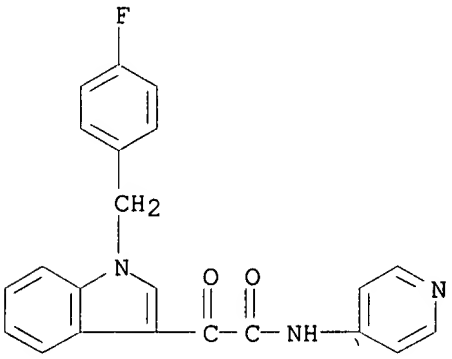

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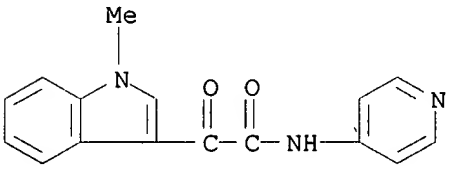

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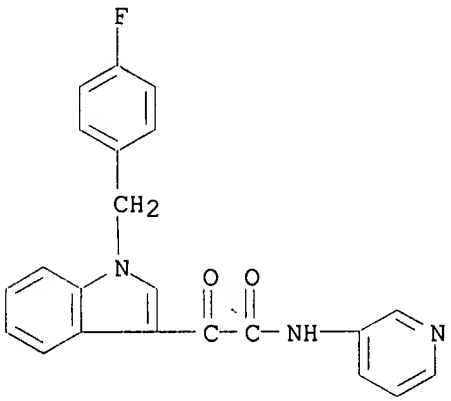
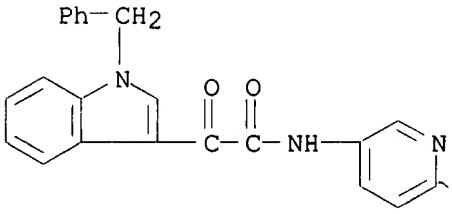


RN 204205-81-2 HCAPLUS
CN 1H-Indole-3-acetamide, .alpha.-oxo-1-(phenylmethyl)-N-3-pyridinyl- (9CI) (CA INDEX NAME)



RN 204205-82-3 HCAPLUS
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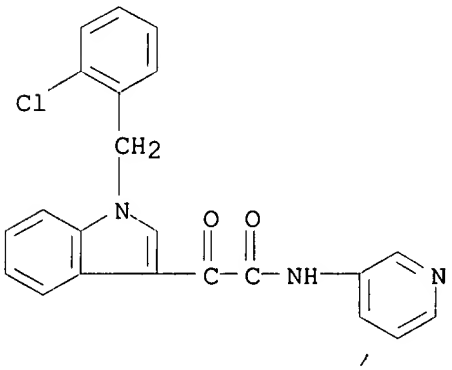

RN 204205-83-4 HCAPLUS
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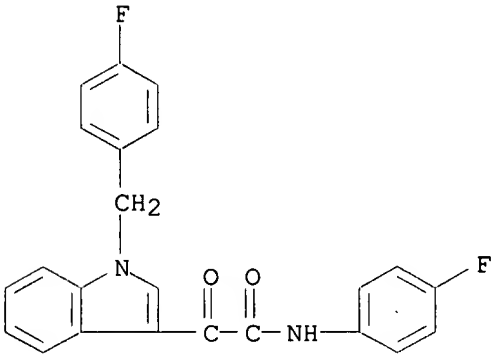

RN 204205-84-5 HCAPLUS
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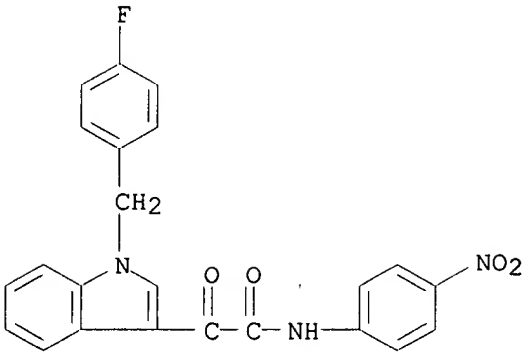

RN 204205-85-6 HCAPLUS
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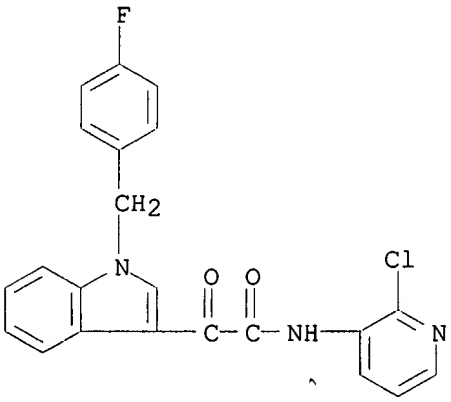

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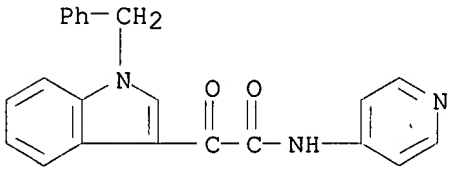

RN 204205-87-8 HCAPLUS
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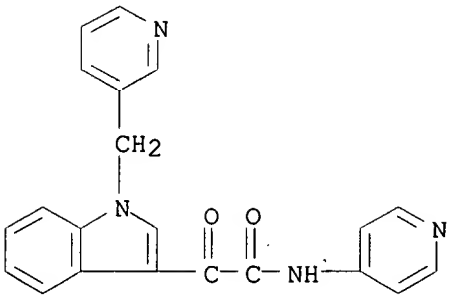

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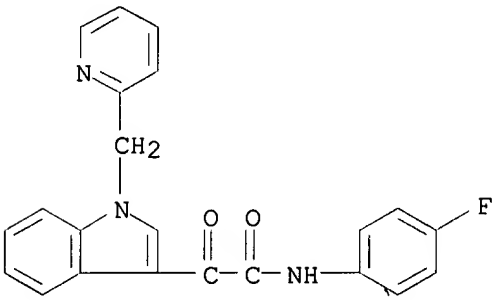

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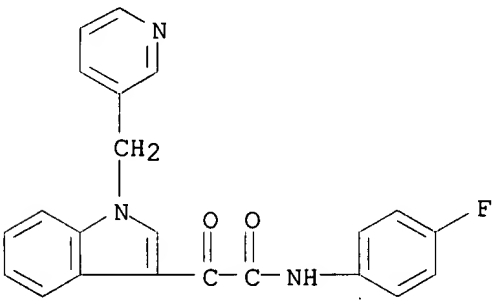

RN 204205-90-3 HCAPLUS
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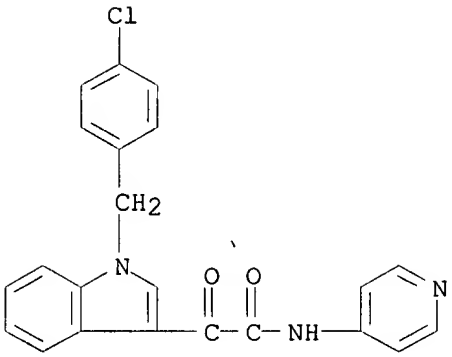

RN 204205-91-4 HCAPLUS
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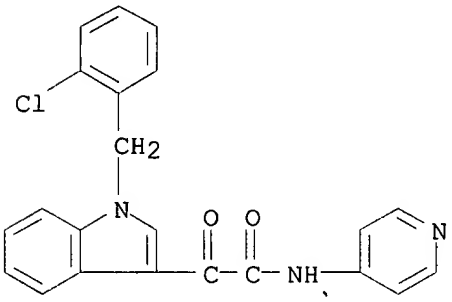
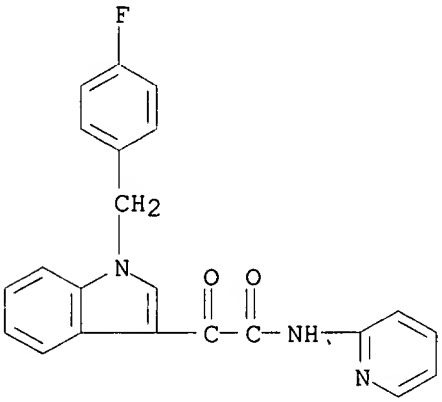
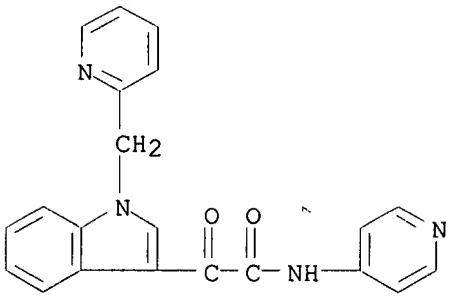


RN 204205-92-5 HCAPLUS
CN 1H-Indole-3-acetamide, 1-[(4-fluorophenyl)methyl]-.alpha.-oxo-N-2-pyridinyl- (9CI) (CA INDEX NAME)



RN 204205-93-6 HCAPLUS
CN 1H-Indole-3-acetamide, .alpha.-oxo-N-4-pyridinyl-1-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 204205-94-7 HCAPLUS
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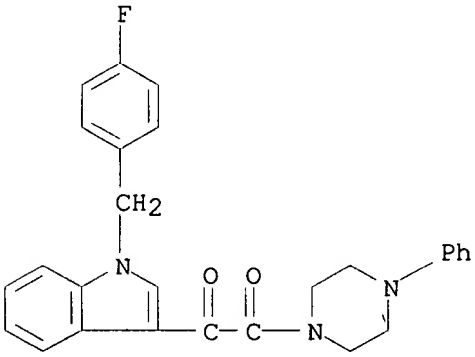

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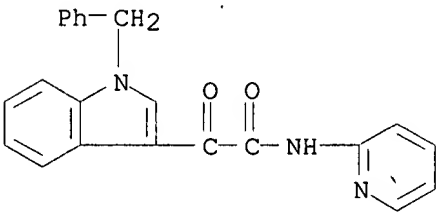
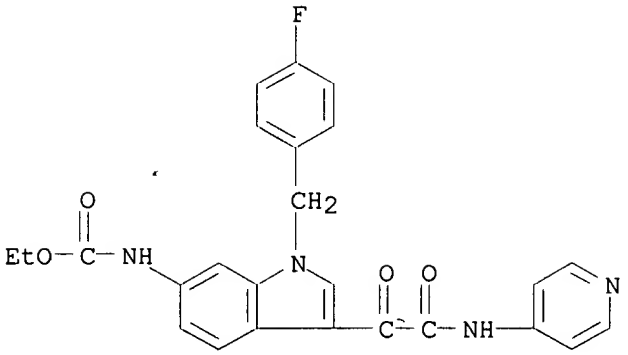
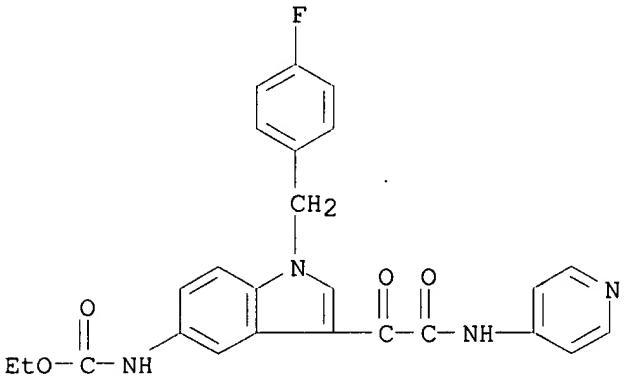


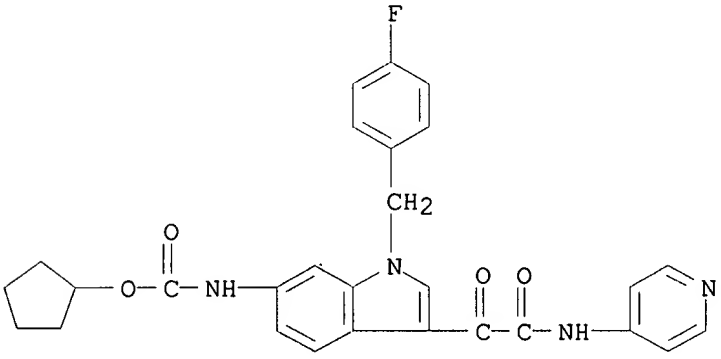
RN 204205-96-9 HCAPLUS
CN Carbamic acid, [1-[(4-fluorophenyl)methyl]-3-[oxo(4-pyridinylamino)acetyl]-1H-indol-6-yl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 204205-97-0 HCAPLUS
CN Carbamic acid, [1-[(4-fluorophenyl)methyl]-3-[oxo(4-pyridinylamino)acetyl]-1H-indol-5-yl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 204205-98-1 HCAPLUS
CN Carbamic acid, [1-[(4-fluorophenyl)methyl]-3-[oxo(4-pyridinylamino)acetyl]-1H-indol-6-yl]-, cyclopentyl ester (9CI) (CA INDEX NAME)



RN 204205-99-2 HCAPLUS
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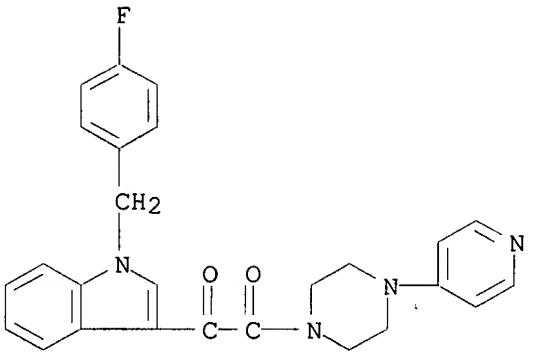
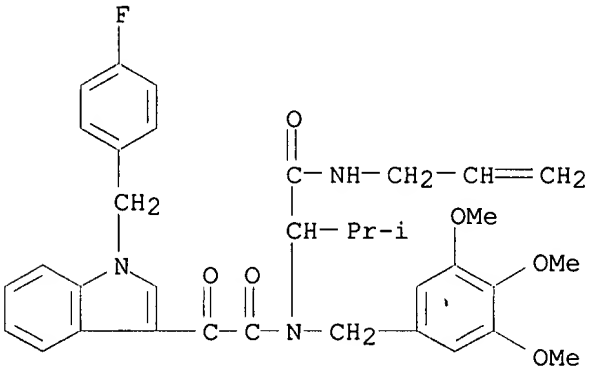


RN 204206-00-8 HCAPLUS
CN 1H-Indole-3-acetamide, 1-[(4-fluorophenyl)methyl]-N-[2-methyl-1-[(2-propenylamino)carbonyl]propyl]-.alpha.-oxo-N-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 204206-01-9 HCAPLUS
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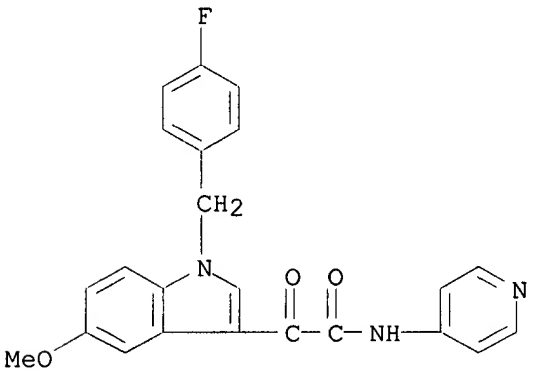

RN 204206-02-0 HCAPLUS
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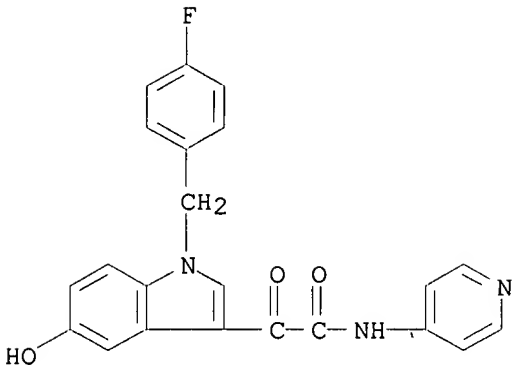

RN 204206-03-1 HCAPLUS
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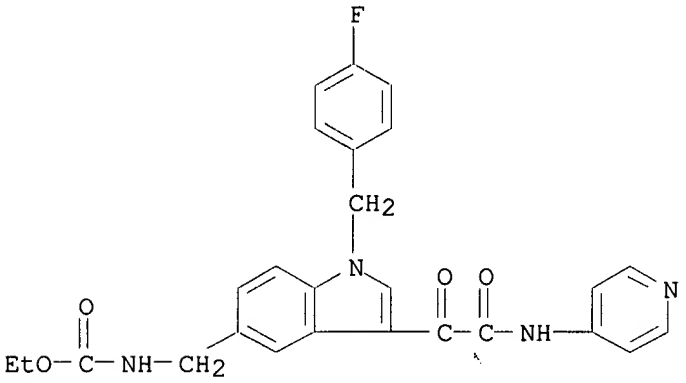

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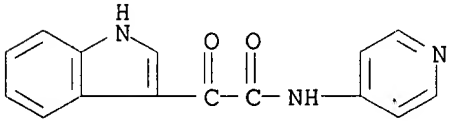

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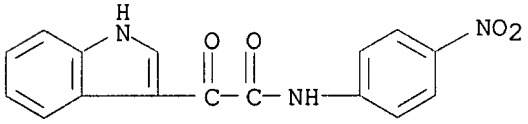

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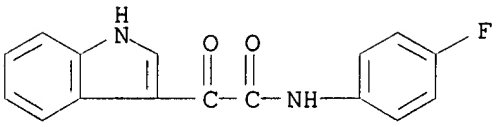
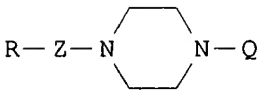
INDEX NAME)



L24 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1997:701490 Document No. 128:22921 Preparation of piperazines having calmodulin inhibitory activity. Yamamoto, Kenjiro; Hasegawa, Atsushi; Kubota, Hideki; Andodeceased, Masahiro; Yamaguchi, Hitoshi (Daiichi Pharmaceutical Co., Ltd., Japan). U.S. US 5681954 A 971028, 44 pp. Cont.-in-part of U.S. Ser. No. 242,842, abandoned. (English). CODEN: USXXAM. APPLICATION: US 95-416311 950404. PRIORITY: JP 93-11277 930514; US 94-242842 940516.

GI



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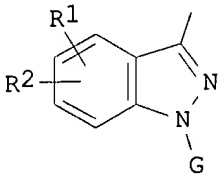

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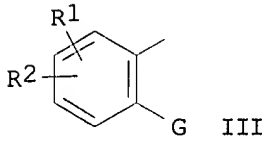
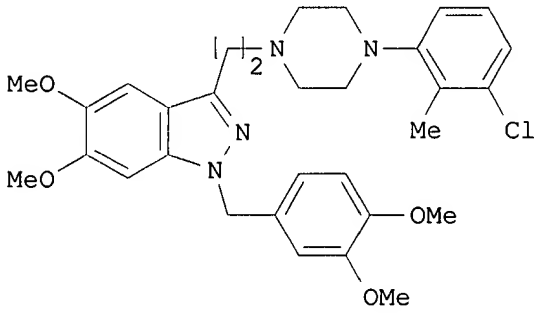


III



IV

AB The title compds. [I; Q = C1-6 alkyl, C1-6 alkoxy, CF3, etc.; R = II or III (wherein G = C1-6 alkyl, (un)substituted Ph, etc.; R1, R2 = C1-6 alkyl, C1-6 alkoxy, CF3, etc.); Z = C1-3 alkylene, C2-4 alkenylene, C(O), etc.], useful as a treating agent for diseases in the circulatory organs or in the cerebral region which are caused by excessive activation of calmodulin, were prepd. Thus, treatment of 1-{[5,6-dimethoxy-1-(3,4-dimethoxybenzyl)-1H-indazol-3-yl]acetyl}-4-(3-chloro-2-methylphenyl)piperazine with BH3*THF in THF afforded the title compd. IV which showed 19.2% increase of survival time on nitrogen-induced hypoxia model in mouse, and IC50 of 3.1 against calmodulin-dependent PDE.

IC ICM C07D413-00
NCL 544114000
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST piperazine prepn calmodulin inhibitor; phosphodiesterase inhibitor calmodulin dependent piperazine prepn; hypoxia piperazine prepn

IT Calmodulins
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of piperazines having calmodulin inhibitory activity)

IT Hypoxia (animal)
(treatment of; prepn. of piperazines having calmodulin inhibitory activity)

IT 9025-82-5, Phosphodiesterase
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(Ca/Calmodulin-dependent PDE inhibitors; prepn. of piperazines having calmodulin inhibitory activity)

IT 160521-99-3P 162495-51-4P 162495-53-6P 198980-94-8P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of piperazines having calmodulin inhibitory activity)

IT 1245-28-9P 4293-90-7P 160521-92-6P 160521-93-7P 162495-33-2P
162495-35-4P 162495-40-1P 162495-41-2P 162495-42-3P
162495-44-5P 162495-48-9P 162495-49-0P 162495-50-3P
162495-52-5P 162495-54-7P 162495-55-8P 162495-91-2P
162495-92-3P 162496-04-0P 162496-06-2P 162496-16-4P
162496-17-5P 162496-18-6P 162496-19-7P 162496-20-0P
162496-23-3P 162496-24-4P 162496-25-5P 162496-27-7P
162496-28-8P 162496-29-9P 162496-30-2P 162496-31-3P
162496-32-4P 162496-33-5P 162496-34-6P 162496-35-7P
162496-38-0P 162496-39-1P 162496-40-4P 162496-41-5P
162496-42-6P 162496-43-7P 162496-44-8P 162496-45-9P
183314-91-2P 183314-93-4P 183314-94-5P 183314-95-6P
183314-96-7P 183314-97-8P 183314-98-9P 183315-01-7P
183315-03-9P 183315-04-0P 183315-05-1P 183315-06-2P
183315-07-3P 183315-08-4P 183315-09-5P 183315-11-9P
183315-13-1P 183315-14-2P 183315-15-3P 183315-16-4P
183315-17-5P 183315-18-6P 183315-19-7P 183315-20-0P
183315-21-1P 183315-22-2P 183315-23-3P 183315-24-4P
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183315-41-5P 183315-45-9P 183315-47-1P 183315-48-2P
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183315-53-9P 183315-84-6P 198980-89-1P 198980-97-1P
198981-00-9P 198981-02-1P 198981-04-3P 198981-05-4P
198981-06-5P 198981-07-6P 198981-08-7P 198981-09-8P
198981-10-1P 198981-11-2P 198981-14-5P 198981-15-6P
198981-16-7P 198981-18-9P 198981-20-3P 198981-22-5P
198981-23-6P 198981-24-7P 198981-26-9P 198981-29-2P
198981-31-6P 198981-32-7P 198981-33-8P 198982-10-4P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of piperazines having calmodulin inhibitory activity)

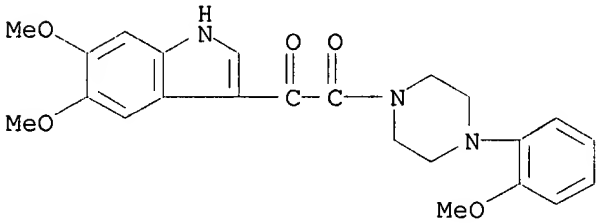
IT 93-07-2, Veratric acid 93-17-4, 3,4-Dimethoxyphenylacetonitrile 93-40-3, 3,4-Dimethoxyphenylacetic acid 105-53-3, Ethyl malonate 109-06-8, 2-Picoline 120-14-9, Veratric aldehyde 120-20-7, 3,4-Dimethoxyphenethylamine 124-68-5, 2-Amino-2-methyl-1-propanol 490-64-2, 2,4,5-Trimethoxybenzoic acid 1207-00-7 1822-51-1, 4-Chloromethylpyridine hydrochloride 4302-52-7, 3,4-Dimethoxyphenylacetylene 4635-59-0, 4-Chlorobutyryl chloride 6315-89-5, 3,4-Dimethoxyaniline 7306-46-9, 3,4-Dimethoxybenzyl chloride 14430-23-0, 5,6-Dimethoxyindole 14794-31-1, Ethyl succinyl chloride 18066-68-7, Ethyl 3,4-dimethoxyphenylacetate 29281-06-9, Ethyl 5,6-dimethoxy-1H-indazole-3-carboxylate 35386-24-4 40255-48-9, 1-(2-Aminoethyl)-4-(2-methoxyphenyl)piperazine 54711-70-5, 1-(3-Chloro-2-

methylphenyl)piperazine 73357-18-3, 4,5-Dimethoxy-2-nitrophenylacetic acid 89980-69-8, 3,4-Dimethoxyphenylmagnesium bromide 98224-26-1, 1-(7-Benzofuranyl)piperazine 103057-10-9, 4-Chloromethyl-1-tritylimidazole 160522-00-9 162496-72-2 162496-73-3 162496-76-6 162496-78-8 162496-79-9 162496-80-2
RL: RCT (Reactant)
(prepn. of piperazines having calmodulin inhibitory activity)

IT 139-76-4P 518-90-1P, Hemipinic acid 569-31-3P, Meconine 1567-56-2P, Hemipinic anhydride 2129-61-5P 5884-22-0P 22248-32-4P 64957-88-6P 68438-33-5P **95442-02-7P** 98205-73-3P 102019-22-7P 104621-47-8P 160521-87-9P 160521-88-0P 160521-89-1P 160521-90-4P 160521-91-5P 160521-94-8P 160521-95-9P 160521-96-0P 160521-97-1P 160521-98-2P 162137-27-1P 162137-44-2P 162496-51-7P 162496-52-8P 162496-54-0P 162496-56-2P 162496-58-4P 162496-60-8P 162496-61-9P 162496-62-0P 162496-63-1P 162496-65-3P 162496-66-4P 162496-67-5P 162496-68-6P 162496-77-7P 183315-86-8P 183315-93-7P 198981-34-9P 198981-35-0P 198981-36-1P 198981-37-2P 198981-38-3P 198981-39-4P 198981-40-7P 198981-41-8P 198981-42-9P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of piperazines having calmodulin inhibitory activity)

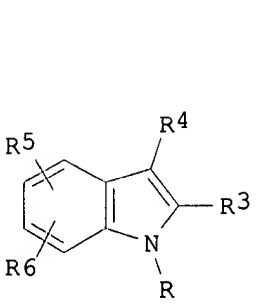
IT **95442-02-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of piperazines having calmodulin inhibitory activity)

RN 95442-02-7 HCAPLUS
CN Piperazine, 1-[(5,6-dimethoxy-1H-indol-3-yl)oxoacetyl]-4-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

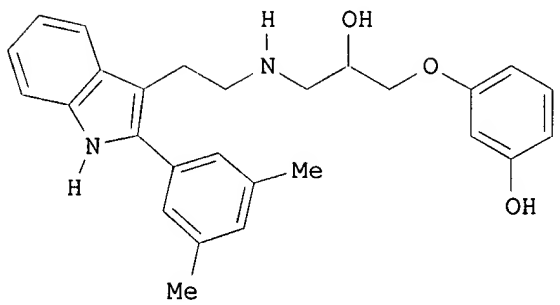


L24 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1997:516361 Document No. 127:121633 Preparation of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists. Goulet, Mark; Bugianesi, Robert L.; Ashton, Wallace T.; Chu, Lin; Fisher, Michael H.; Lin, Peter; Smith, Roy G.; Ponpipom, Mitree M.; Wyvratt, Matthew J.; Yang, Yi Tien (Merck & Co., Inc., USA; Goulet, Mark; Bugianesi, Robert L.; Ashton, Wallace T.; Chu, Lin; Fisher, Michael H.; Lin, Peter; Smith, Roy G.; Ponpipom, Mitree M.; et al.). PCT Int. Appl. WO 9721435 A1 970619, 147 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 96-US20004 961210. PRIORITY: US 95-8632 951214; GB 96-3370 960216.

GI



I



II

AB Title compds. [I; R = H, (ar)alkyl, aryl, etc.; R3 = (un)substituted Ph; R4 = (CR9R9a)m CR10R10aNR2ZR1; R1 = (un)substituted Ph, -naphthyl, -biphenylyl, etc.; R2 = H, (ar)alkyl, aryl, etc.; R5 = H, halo, OR7, OR8, NR7R8, COR7, COR8, etc.; R6 = H, halo, (perfluoro)alkyl, aryl, etc.; R7 = H or (un)substituted alkyl; R9,R9a = H, (ar)alkyl, aryl, etc.; R10,R10a = H, (ar)alkyl, aryl, etc.; Z = (un)substituted alk(en)ylene, etc.; NR2Z = heterocyclene; m = 0-3] were prepd. as gonadotropin releasing hormone antagonists (no data). Thus, indole-3-ethanamine was N-protected and the brominated product arylated with 3,5-Me2C6H3B(OH)2 to give, after deprotection, 2-(3,5-dimethylphenyl)indole-3-ethanamine which was condensed with 3-benzyloxyphenyl glycidyl ether to give, after deprotection, title compd. II.

IC ICM A61K031-40
ICS C07D209-14

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 2

ST arylindolealkanamine prepn gonadotropin releasing hormone antagonist

IT Gonadotropin-releasing hormone receptor
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(inhibitors; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 107950-52-7, Gonadotropin-releasing hormone
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(mediated diseases; treatment; prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 192770-97-1P 192771-89-4P 192773-06-1P 192773-09-4P
192773-15-2P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 192770-78-8P 192770-79-9P 192770-80-2P 192770-81-3P
192770-82-4P 192770-83-5P 192770-84-6P 192770-85-7P
192770-86-8P 192770-87-9P 192770-88-0P 192770-89-1P
192770-90-4P 192770-91-5P 192770-92-6P 192770-93-7P
192770-94-8P 192770-95-9P 192770-96-0P 192770-98-2P
192770-99-3P 192771-00-9P 192771-01-0P 192771-02-1P
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192771-31-6P 192771-32-7P 192771-33-8P 192771-34-9P
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192771-43-0P 192771-44-1P 192771-45-2P 192771-46-3P
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192771-67-8P 192771-68-9P 192771-69-0P 192771-70-3P
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192771-75-8P 192771-76-9P 192771-77-0P 192771-78-1P
192771-79-2P 192771-80-5P 192771-81-6P 192771-82-7P
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192771-87-2P 192771-88-3P 192771-90-7P 192771-91-8P
192771-92-9P 192771-93-0P 192771-94-1P 192771-95-2P
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192772-00-2P 192772-01-3P 192772-02-4P 192772-03-5P
192772-04-6P 192772-05-7P 192772-06-8P 192772-07-9P
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192772-94-4P 192772-95-5P 192772-96-6P 192772-97-7P
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192773-02-7P 192773-03-8P 192773-04-9P 192773-05-0P
192773-07-2P 192773-08-3P 192773-10-7P 192773-11-8P
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192773-17-4P 192773-18-5P 192773-19-6P 192773-20-9P
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192773-25-4P 192773-26-5P 192773-27-6P 192773-28-7P
192773-29-8P 192773-30-1P 192773-31-2P 192773-32-3P
192773-33-4P 192773-34-5P 192773-35-6P 192773-36-7P
192773-37-8P 192773-38-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 192773-39-0P 192773-40-3P 192773-41-4P 192773-42-5P
192773-43-6P 192773-44-7P 192773-45-8P 192773-46-9P
192773-47-0P 192773-48-1P 192773-49-2P 192773-50-5P
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192773-83-4P 192773-84-5P 192773-85-6P 192773-86-7P
192773-87-8P 192773-88-9P 192773-89-0P 192773-90-3P

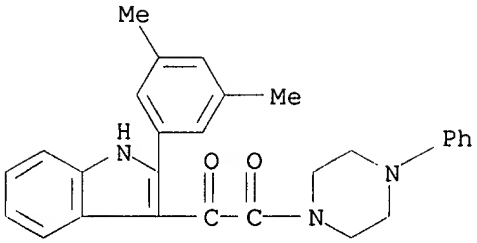
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 61-54-1, 1H-Indole-3-ethanamine 79-44-7, Dimethylcarbamyl chloride 92-54-6, 1-Phenylpiperazine 100-39-0, Benzyl bromide 104-03-0, 4-Nitrophenylacetic acid 107-10-8, 1-Propanamine, reactions 108-18-9, Diisopropylamine 109-89-7, Diethylamine, reactions 501-53-1, Benzyl chloroformate 501-97-3, 3-(4-Hydroxyphenyl)propionic acid 556-96-7, 5-Bromo-m-xylene 619-67-0, 4-Hydrazinobenzoic acid 4635-59-0, 4-Chlorobutyryl chloride 5438-70-0, Ethyl 4-aminophenylacetate 5600-62-4, 4-(4-Nitrophenyl)butyric acid 6293-83-0, 2-Iodo-4-nitroaniline 6366-06-9, 3,5-Dimethylphenylacetylene 13436-46-9, 2-Ethoxytetrahydrofuran 19910-33-9, 2-(4-Nitrophenyl)propionic acid 20776-45-8, 5-Benzyloxytryptamine 22205-09-0, 4-(4-Aminobutyl)phenol 22509-74-6, N-Ethoxycarbonylphthalimide 29555-02-0, 2-Methylcyclopropanecarboxylic acid 34674-93-6, 4-(4-Hydroxyphenyl)butyric acid 53672-98-3 95426-76-9 96090-12-9 105640-07-1 192717-25-2 192774-26-8 192774-27-9
RL: RCT (Reactant)
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

IT 6686-26-6P 15741-71-6P 19571-34-7P 36924-81-9P, Ethyl 2-(4-aminophenyl)-2-methylpropionate 50712-64-6P, Ethyl 2-(4-Nitrophenyl)propionate 53157-45-2P 64214-66-0P 65476-32-6P 79606-42-1P 79606-48-7P 83397-45-9P 137402-61-0P 150668-36-3P 172975-69-8P, 3,5-Dimethylphenylboronic acid 192182-01-7P 192182-34-6P 192182-46-0P 192182-48-2P 192643-78-0P 192643-86-0P 192643-90-6P 192644-20-5P 192644-21-6P 192717-28-5P 192770-58-4P 192770-59-5P 192770-60-8P 192770-62-0P 192770-63-1P 192770-65-3P 192770-66-4P 192770-67-5P 192770-69-7P 192770-70-0P 192770-71-1P 192770-72-2P 192770-73-3P 192770-74-4P 192770-75-5P 192770-76-6P 192770-77-7P 192773-91-4P 192773-92-5P 192773-93-6P 192773-94-7P 192773-95-8P 192773-96-9P 192773-97-0P 192773-98-1P 192773-99-2P 192774-00-8P 192774-01-9P 192774-02-0P 192774-03-1P 192774-04-2P 192774-05-3P 192774-06-4P 192774-07-5P 192774-08-6P 192774-09-7P 192774-10-0P 192774-11-1P 192774-12-2P 192774-13-3P 192774-14-4P 192774-15-5P 192774-16-6P 192774-17-7P 192774-18-8P 192774-19-9P 192774-20-2P 192774-21-3P, 4-Hydrazino-N,N-diisopropylbenzamide 192774-22-4P 192774-23-5P 192774-24-6P **192774-25-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

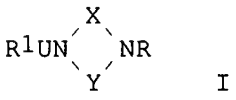
IT **192774-25-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of N-aralkyl-2-arylindole-3-alkanamines and analogs as gonadotropin releasing hormone antagonists)

RN 192774-25-7 HCAPLUS
CN Piperazine, 1-[[2-(3,5-dimethylphenyl)-1H-indol-3-yl]oxoacetyl]-4-phenyl- (9CI) (CA INDEX NAME)

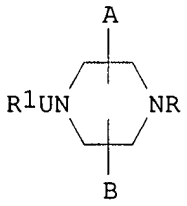


L24 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1997:499179 Document No. 127:176441 Preparation of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides.. Silverman, Ian R.; Ali, Syed F.; Cohen, Daniel H.; Lyga, John W.; Simmons, Kirk A.; Cullen, Thomas G. (FMC Corp., USA). PCT Int. Appl. WO 9726252 A1 970724, 59 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 97-US804 970115. PRIORITY: US 96-10237 960119; US 97-780371 970109.

GI



I



II

AB Title compds. [I; A, B = alkyl; U = alkylene, alkenylene, CHZ; Z = H, alkyl, cycloalkyl, Ph; R = (substituted) Ph, dibenzocycloalkyl, etc.; R1 = (substituted) Ph, naphthyl, tetrazolylphenyl, benzothienyl, benzimidazolyl, indolyl, pyrrolyl, quinolinyl, etc.; X = (CH2)m; Y = (CH2)n; m = 2,3; n = 1-3], were prepd. Thus, reaction of N-[bis(4-trifluoromethylphenyl)methyl]piperazine and 4-(pyrid-2-yloxy)benzyl chloride in Me2SO contg. NaI and diisopropylethylamine gave N-[4-(pyrid-2-yloxy)phenylmethyl]-N'-[bis(4-trifluoromethylphenyl)methyl]piperazine. The latter at 50 micromolar in feed gave 100% inhibition of the growth of tobacco budworms.

IC ICM C07D295-033
ICS C07D295-096; C07D295-135; C07D295-192; C07D401-06; C07D403-06; C07D405-12; C07D409-06; C07D417-12

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

ST heterocyclylalkylpiperazine prepn insecticide; piperazine heterocyclylalkyl prepn insecticide

IT Insecticides
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

IT 194016-31-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector,

except adverse); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

IT 298-57-7P 16896-82-5P 49853-47-6P 101477-55-8P 112292-03-2P
112292-13-4P 112292-15-6P 114951-24-5P 115688-90-9P
194016-15-4P 194016-16-5P 194016-17-6P 194016-18-7P
194016-19-8P 194016-20-1P 194016-21-2P 194016-22-3P
194016-23-4P 194016-24-5P 194016-25-6P 194016-26-7P
194016-27-8P 194016-28-9P 194016-29-0P 194016-30-3P
194016-32-5P 194016-33-6P 194016-34-7P 194016-35-8P
194016-36-9P 194016-37-0P 194016-38-1P 194016-39-2P
194016-40-5P 194016-41-6P 194016-42-7P 194016-43-8P
194016-44-9P 194016-45-0P 194016-46-1P 194016-47-2P
194016-48-3P 194016-49-4P 194016-50-7P 194016-51-8P
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194016-68-7P 194016-69-8P 194016-70-1P 194016-71-2P
194016-72-3P 194016-73-4P 194016-74-5P 194016-75-6P
194016-76-7P 194016-77-8P 194016-78-9P 194016-79-0P
194016-80-3P 194016-81-4P 194016-82-5P 194016-83-6P
194016-84-7P 194016-85-8P 194016-86-9P 194016-87-0P
194016-88-1P 194016-89-2P 194016-90-5P 194016-91-6P
194016-92-7P 194016-93-8P 194016-94-9P 194016-95-0P
194016-96-1P 194016-97-2P 194016-98-3P 194017-00-0P
194017-01-1P 194017-02-2P 194017-03-3P 194017-04-4P
194017-05-5P **194017-06-6P** 194017-07-7P 194017-08-8P
194017-09-9P 194017-10-2P 194017-11-3P 194017-12-4P
194017-13-5P 194017-14-6P 194017-15-7P 194017-16-8P
194017-17-9P 194017-18-0P 194017-19-1P 194017-20-4P
194017-21-5P 194017-22-6P 194017-23-7P 194017-24-8P
194017-25-9P 194017-26-0P 194017-27-1P 194017-28-2P
194017-29-3P 194017-30-6P 194017-31-7P 194017-32-8P
194017-33-9P 194017-34-0P 194017-35-1P 194017-36-2P
194017-37-3P 194017-38-4P 194017-39-5P 194017-40-8P
194017-41-9P 194017-42-0P 194017-43-1P 194017-44-2P
194017-45-3P 194017-46-4P 194017-47-5P 194017-48-6P
194017-49-7P 194017-50-0P 194017-51-1P 194017-52-2P
194017-53-3P 194017-54-4P 194017-55-5P 194017-56-6P
194017-57-7P 194017-58-8P 194017-59-9P 194017-60-2P
194017-72-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

IT 85-29-0, 2,4'-Dichlorobenzophenone 100-59-4, Phenylmagnesium chloride 104-85-8, 4-Cyanotoluene 109-94-4, Ethyl formate 110-85-0, Piperazine, reactions 120-43-4, Ethyl 1-piperazinecarboxylate 123-08-0 123-38-6, Propionaldehyde, reactions 303-26-4 372-48-5, 2-Fluoropyridine 402-43-7, 4-Bromobenzotrifluoride 455-19-6, 4-Trifluoromethylbenzaldehyde 586-75-4, 4-Bromobenzoyl chloride 762-49-2, 1-Bromo-2-fluoroethane 1507-90-0 1912-43-2, 2-Methylindole-3-acetic acid 25235-85-2, 4-Chloroindole 27469-60-9
RL: RCT (Reactant)
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

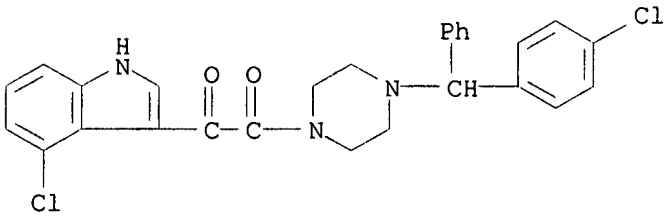
IT 876-72-2P 22543-52-8P 24994-04-5P 42498-38-4P 43171-49-9P
97027-84-4P 104523-03-7P 104523-09-3P 112809-57-1P
112809-58-2P 194017-61-3P 194017-62-4P 194017-63-5P
194017-64-6P 194017-65-7P 194017-66-8P 194017-67-9P

194017-68-0P 194017-69-1P 194017-70-4P 194017-71-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

IT **194017-06-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of N-heterocyclylalkyl- or N-[(polycyclyl)-alkyl]-N'-substituted piperazines as insecticides)

RN 194017-06-6 HCAPLUS

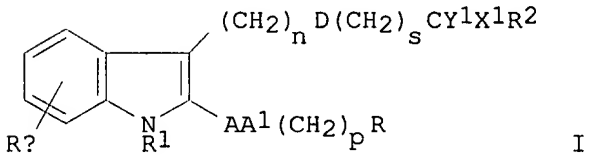
CN Piperazine, 1-[(4-chloro-1H-indol-3-yl)oxoacetyl]-4-[(4-chlorophenyl)phenylmethyl]- (9CI) (CA INDEX NAME)



L24 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 1998 ACS

1997:293836 Document No. 126:264004 Preparation and formulation of indole derivatives as neuropeptide Y receptor antagonists. Britton, Thomas C.; Bruns, Robert F., Jr; Gehlert, Donald R.; Hipskind, Philip A.; Lobb, Karen L.; Nixon, James A.; Ornstein, Paul L.; Smith, Edward C. R.; Zarrinmayeh, Hamideh; Zimmerman, Dennis M. (Lilly, Eli, and Co., USA). PCT Int. Appl. WO 9709308 A1 970313, 309 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 96-US14163 960830. PRIORITY: US 95-3150 950901; GB 95-23999 951123; US 96-21638 960712.

GI



I

AB The title compds. I [Ra = H, alkyl, etc.; R1 = H, alkyl, etc.; A = bond, CO, etc.; A1 = bond, O, etc.; n, p, s = 0 - 6; D = bond, etc.; one of X1 and Y1 is hydroxy and the other is hydrogen; or both X1 and Y1 are hydrogen, or X1 and Y1 combine to form oxo, etc.; R2 = OH, etc.; R = Ph, etc.] are prepd. I are useful in treating or preventing a condition assocd. with an excess of neuropeptide Y. Many of the compds. of this invention are said to show significant activity as neuropeptide Y receptor antagonists (Ki = 10 .mu.M to 0.1 nM).

IC ICM C07D209-04
ICS A61K031-34

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
ST indole prepn neuropeptide antagonist
IT Receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(prepn. and formulation of indole derivs. with effect on neuropeptide Y receptors)
IT 76869-06-2P 81095-89-8P 102313-73-5P 188720-57-2P
188720-58-3P 188720-59-4P 188720-60-7P 188720-61-8P
188720-62-9P 188720-63-0P 188720-64-1P 188720-65-2P
188720-66-3P 188720-67-4P 188720-68-5P 188720-69-6P
188720-70-9P 188720-71-0P 188720-72-1P 188720-73-2P
188720-74-3P 188720-75-4P 188720-76-5P 188720-77-6P
188720-78-7P 188720-79-8P 188720-80-1P 188720-81-2P
188720-82-3P 188720-83-4P 188720-84-5P 188720-85-6P
188720-86-7P 188720-87-8P 188720-88-9P 188720-89-0P
188720-90-3P 188720-91-4P 188720-92-5P 188720-93-6P
188720-94-7P 188720-95-8P 188720-96-9P 188720-97-0P
188720-98-1P 188720-99-2P 188721-00-8P 188721-01-9P
188721-02-0P 188721-03-1P 188721-04-2P 188721-05-3P
188721-06-4P 188721-07-5P 188721-08-6P 188721-09-7P
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188721-14-4P 188721-15-5P 188721-16-6P 188721-17-7P
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188721-22-4P 188721-23-5P 188721-24-6P 188721-25-7P
188721-26-8P 188721-27-9P 188721-28-0P 188721-29-1P
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188721-61-1P 188721-63-3P 188721-65-5P 188721-66-6P
188721-67-7P **188721-68-8P 188721-69-9P**
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188721-89-3P 188721-90-6P 188721-91-7P 188721-92-8P
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188721-97-3P 188721-98-4P 188721-99-5P 188722-00-1P
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188722-13-6P 188722-14-7P 188722-15-8P 188722-16-9P
188722-17-0P 188722-18-1P 188722-19-2P 188722-20-5P
188722-21-6P 188722-22-7P 188722-23-8P 188722-24-9P
188722-25-0P 188722-26-1P 188722-27-2P 188722-28-3P
188722-29-4P 188722-30-7P 188722-31-8P 188722-32-9P
188722-33-0P 188722-34-1P 188722-35-2P 188722-36-3P
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188722-41-0P 188722-42-1P 188722-43-2P 188722-44-3P
188722-46-5P 188722-48-7P 188722-50-1P 188722-51-2P
188722-52-3P 188722-53-4P 188722-54-5P 188722-55-6P
188722-56-7P 188722-57-8P 188722-58-9P 188722-59-0P
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188722-64-7P 188722-65-8P 188722-66-9P 188722-67-0P
188722-68-1P 188722-69-2P 188722-70-5P 188722-71-6P
188722-72-7P 188722-73-8P 188722-74-9P 188722-75-0P
188722-76-1P 188722-77-2P 188722-78-3P 188722-80-7P
188722-82-9P 188722-83-0P 188722-84-1P 188722-85-2P

188722-86-3P 188722-87-4P 188722-88-5P 188722-89-6P
188722-90-9P 188722-91-0P 188722-92-1P 188722-93-2P
188722-94-3P 188722-95-4P 188722-96-5P 188722-97-6P
188722-98-7P
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)

IT 188722-99-8P 188723-00-4P 188723-01-5P 188723-02-6P
188723-04-8P 188723-06-0P 188723-07-1P 188723-08-2P
188723-09-3P 188723-10-6P 188723-11-7P 188723-12-8P
188723-13-9P 188723-14-0P 188723-15-1P 188723-16-2P
188723-17-3P 188723-18-4P 188723-19-5P 188723-20-8P
188723-21-9P 188723-22-0P 188723-23-1P 188723-24-2P
188723-25-3P 188723-26-4P 188723-27-5P 188723-28-6P
188723-29-7P 188723-30-0P 188723-31-1P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)

IT 75-31-0, Isopropylamine, reactions 75-64-9, reactions 79-37-8, Oxalyl chloride 92-54-6, Phenylpiperazine 110-91-8, Morpholine, reactions 115-11-7, reactions 124-38-9, Carbon dioxide, reactions 352-33-0, 1-Chloro-4-fluorobenzene 500-22-1, 3-Pyridine carboxaldehyde 611-71-2 626-58-4, 4-Methylpiperidine 1066-54-2, (Trimethylsilyl)acetylene 4897-50-1, 4-(Piperidino)piperidine 6711-48-4 16136-58-6 16246-98-3 17199-29-0, L-Mandelic acid 24424-99-5 30525-89-4, Paraformaldehyde 39931-77-6, Ethyl-3-pyridylacetate 188724-14-3 188724-15-4 188724-17-6
RL: RCT (Reactant)
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)

IT 394-30-9P 1202-04-6P 1485-22-9P 28447-17-8P 42042-71-7P 64977-30-6P 71916-91-1P 75717-77-0P 91017-00-4P 99725-12-9P 111300-06-2P 153039-16-8P 179419-05-7P 188723-32-2P
188723-33-3P 188723-34-4P 188723-35-5P 188723-36-6P
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188723-49-1P 188723-50-4P 188723-51-5P 188723-53-7P
188723-54-8P 188723-55-9P 188723-56-0P 188723-57-1P
188723-58-2P 188723-59-3P 188723-60-6P 188723-61-7P
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188723-66-2P 188723-67-3P 188723-68-4P 188723-69-5P
188723-70-8P 188723-71-9P 188723-72-0P 188723-73-1P
188723-74-2P 188723-75-3P 188723-76-4P 188723-77-5P
188723-78-6P 188723-79-7P 188723-80-0P 188723-81-1P
188723-82-2P 188723-83-3P 188723-84-4P 188723-85-5P
188723-86-6P 188723-89-9P 188723-91-3P 188723-92-4P
188723-93-5P 188723-94-6P 188723-95-7P 188723-96-8P
188723-97-9P 188723-98-0P 188723-99-1P 188724-00-7P
188724-01-8P 188724-02-9P 188724-03-0P 188724-04-1P
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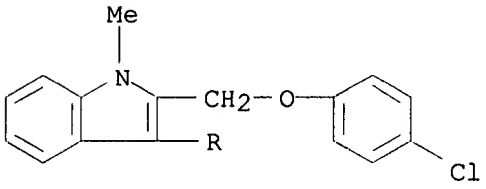
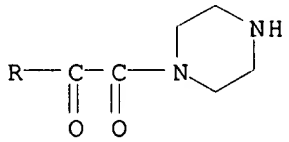
188724-09-6P 188724-10-9P 188724-11-0P 188724-12-1P
188724-13-2P 188883-57-0P 188883-58-1P 188883-59-2P
188883-60-5P 188883-61-6P 188883-62-7P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)

IT **188721-68-8P 188721-69-9P 188721-70-2P**

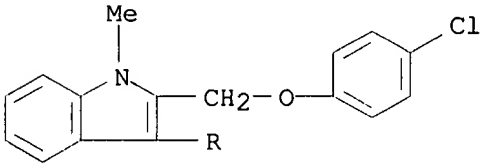
188721-71-3P 188721-72-4P
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)

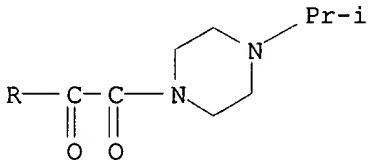
RN 188721-68-8 HCAPLUS
CN Piperazine, 1-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)



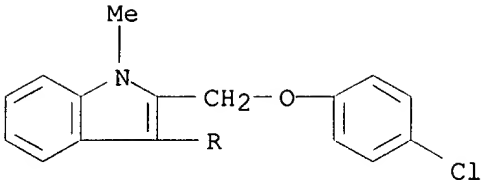


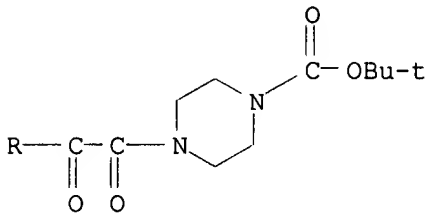
RN 188721-69-9 HCAPLUS
CN Piperazine, 1-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



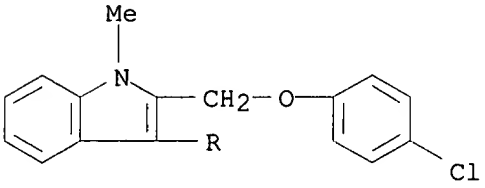


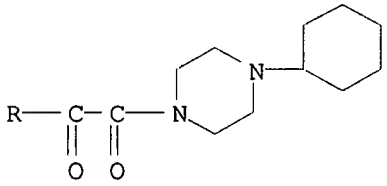
RN 188721-70-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



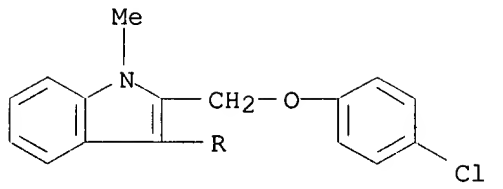


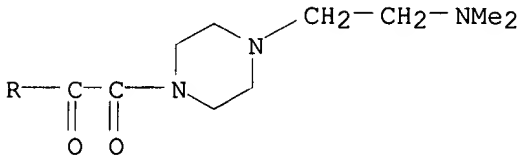
RN 188721-71-3 HCAPLUS
CN Piperazine, 1-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]-4-cyclohexyl- (9CI) (CA INDEX NAME)





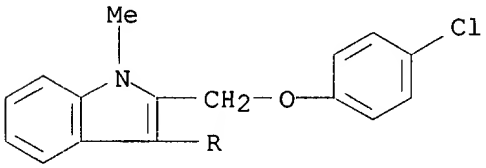
RN 188721-72-4 HCAPLUS
CN 1-Piperazineethanamine, 4-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)

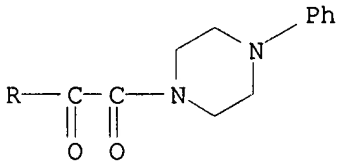




● 2 HCl

IT **188723-37-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and formulation of indole derivs. as neuropeptide Y receptor antagonists)
RN 188723-37-7 HCAPLUS
CN Piperazine, 1-[[2-[(4-chlorophenoxy)methyl]-1-methyl-1H-indol-3-yl]oxoacetyl]-4-phenyl- (9CI) (CA INDEX NAME)





L24 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1996:713055 Document No. 126:69723 Synthesis, structure-activity relationships, and molecular modeling studies of N-(indol-3-ylglyoxylyl)benzylamine derivatives acting at the benzodiazepine receptor. Da Settimo, Antonio; Primofiore, Giampaolo; Da Settimo, Federico; Marini, Anna Maria; Novellino, Ettore; Greco, Giovanni; Martini, Claudia; Giannaccini, Gino; Lucacchini, Antonio (Dipartimento di Scienze Farmaceutiche, Universita di Pisa, Pisa, 56126, Italy). J. Med. Chem., 39(26), 5083-5091 (English) 1996. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical Society.
AB A no. of N-(indol-3-ylglyoxylyl)benzylamine derivs. were synthesized and tested for [3H]flunitrazepam displacing activity in bovine brain membranes. Some of these derivs. exhibited high affinity for the

benzodiazepine receptor (BzR) with Ki values ranging from 67 to 11 nM. The GABA ratio and [35S]-tert-butylbicyclophosphorothionate binding data, detd. for the most active compds., showed that they elicit an efficacy profile at the BzR which depends on the kind of substituent present on the Ph ring of the benzylamine moiety. Moreover, lengthening (propylamine derivs.) and shortening (aniline derivs.) of the distance between the Ph ring and the amide group of the side chain gave compds. with a drastically lower binding potency. The biol. results are discussed in the light of a recently proposed pharmacophore model and compared, by mol. modeling studies, with those obtained from effective BzR ligands.

CC 1-3 (Pharmacology)
Section cross-reference(s): 27

ST indolylglyoxylyl benzylamine deriv benzodiazepine receptor binding; structure activity synthesis indolylglyoxylyl benzylamine

IT Receptor-binding structure-activity relationship
(benzodiazepine receptor-binding; synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT Anticonvulsants
Biological simulation
Brain
Convulsions
Pharmacophores
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT Benzodiazepine receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT Amines, reactions
RL: RCT (Reactant)
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT 439-14-5, Diazepam
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT 61-38-1P 61-39-2P 55654-71-2DP, derivs. 55654-71-2P
73031-16-0P 149167-36-2P 149167-37-3P 149167-38-4P
149167-39-5P 149167-40-8P 149167-41-9P 149167-42-0P
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149167-47-5P 149167-48-6P 149167-49-7P 149167-50-0P
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149167-59-9P 149167-60-2P 149167-61-3P 149167-62-4P
185391-17-7P 185391-22-4P 185391-24-6P 185391-26-8P
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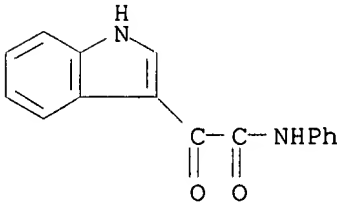
185391-39-3P 185391-41-7P 185391-43-9P 185391-45-1P
185391-47-3P 185391-49-5P 185391-57-5P **185391-63-3P**
185391-65-5P 185391-67-7P 185391-69-9P
185391-71-3P 185391-73-5P 185391-75-7P
185391-76-8P
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

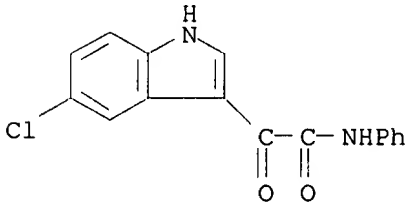
IT 22980-09-2
RL: RCT (Reactant)
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

IT **73031-16-0P 185391-63-3P 185391-65-5P 185391-67-7P 185391-69-9P 185391-71-3P 185391-73-5P 185391-75-7P 185391-76-8P**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(synthesis, structure-activity relationships, and mol. modeling of N-(indol-3-ylglyoxylyl)benzylamine derivs. acting at benzodiazepine receptor)

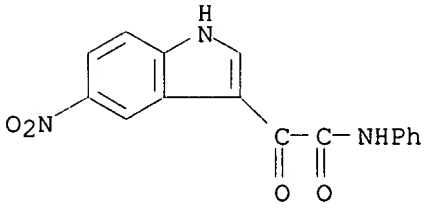
RN 73031-16-0 HCAPLUS
CN 1H-Indole-3-acetamide, .alpha.-oxo-N-phenyl- (9CI) (CA INDEX NAME)



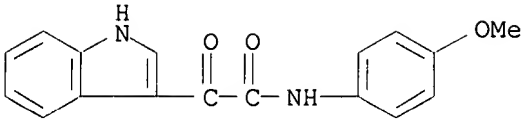
RN 185391-63-3 HCAPLUS
CN 1H-Indole-3-acetamide, 5-chloro-.alpha.-oxo-N-phenyl- (9CI) (CA INDEX NAME)



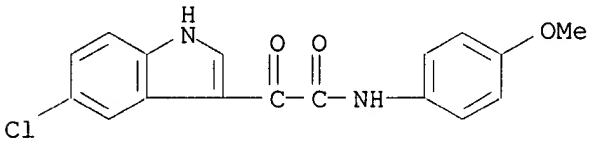
RN 185391-65-5 HCAPLUS
CN 1H-Indole-3-acetamide, 5-nitro-.alpha.-oxo-N-phenyl- (9CI) (CA INDEX NAME)



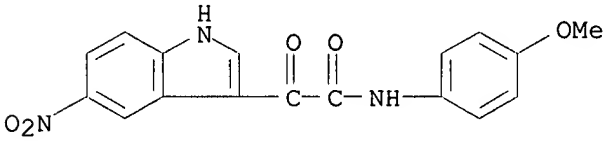
RN 185391-67-7 HCAPLUS
CN 1H-Indole-3-acetamide, N-(4-methoxyphenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



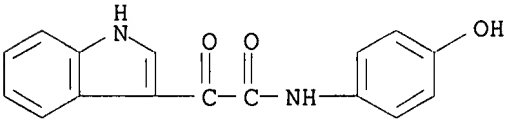
RN 185391-69-9 HCAPLUS
CN 1H-Indole-3-acetamide, 5-chloro-N-(4-methoxyphenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



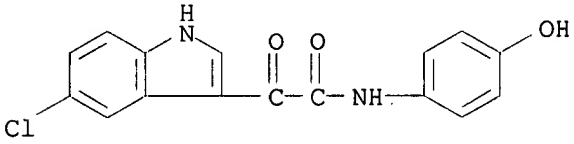
RN 185391-71-3 HCAPLUS
CN 1H-Indole-3-acetamide, N-(4-methoxyphenyl)-5-nitro-.alpha.-oxo- (9CI) (CA INDEX NAME)



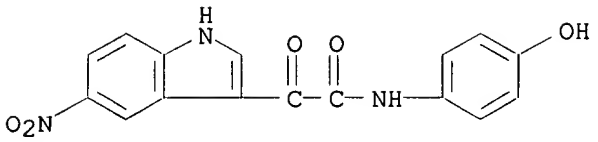
RN 185391-73-5 HCAPLUS
CN 1H-Indole-3-acetamide, N-(4-hydroxyphenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



RN 185391-75-7 HCAPLUS
CN 1H-Indole-3-acetamide, 5-chloro-N-(4-hydroxyphenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



RN 185391-76-8 HCAPLUS
CN 1H-Indole-3-acetamide, N-(4-hydroxyphenyl)-5-nitro-.alpha.-oxo- (9CI) (CA INDEX NAME)



L24 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1996:681493 Document No. 126:42242 Development of Potent Thrombin Receptor Antagonist Peptides. Bernatowicz, Michael S.; Klimas, Clifford E.; Hartl, Karen S.; Peluso, Marianne; Allegretto, Nick J.; Seiler, Steven M. (Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA). J. Med. Chem., 39(25), 4879-4887 (English) 1996. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical Society.

AB A peptide-based structure-activity study is reported leading to the discovery of novel potent thrombin receptor antagonists. Systematic substitution of nonproteogenic amino acids for the 2nd and 3rd residues of the human thrombin receptor tethered ligand sequence (SFLLR) led to a series of agonists with enhanced potency. The most potent pentapeptide agonist identified was Ser-p-fluoroPhe-p-guanidinoPhe-Leu-Arg-NH2 (I) (EC50 .apprx.0.04 .mu.M for stimulation of human platelet aggregation, .apprx.10-fold more potent than the natural pentapeptide). Systematic substitution of the NH2-terminal Ser in I with neutral hydrophobic NH2-acyl groups led to partial agonists and eventually antagonists with unprecedented potency (>1000-fold increase over the previously reported antagonist 3-mercaptopropionyl-Phe-Cha-Cha-Arg-Lys-Pro-Asn-Asp-Lys-NH2). In the series of NH2-acyl tetrapeptide antagonists, N-trans-cinnamoyl-p-fluoroPhe-p-guanidinoPhe-Leu-Arg-NH2 (II) was identified as the tightest binding (IC50 .apprx.8 nM) and most potent with an IC50 .apprx.0.20 .mu.M for inhibition of SFLLRNP-NH2-stimulated platelet aggregation. Systematic single substitutions in (II) indicated that, in addn. to the NH2-terminal acyl group, the side chains at the 2nd and 3rd positions were also responsible for important and specific receptor interactions. The p-fluoroPhe and p-guanidinoPhe residues in the 2nd and 3rd positions of II were obsd. to be optimal in both the agonist and antagonist series. In the case of antagonists, however, an appropriately positioned pos. charged group (i.e., protonated base) at the 3rd residue was required. In contrast, such a substitution was not required for potent agonist activity. An even more potent antagonist resulted when II was extended at the C-terminus by a single Arg residue giving rise to analog BMS-200261 (III) which had an IC50 .apprx.20 nM for inhibition of SFLLRNP-NH2-stimulated platelet aggregation. When the C-terminal Arg of III was replaced by an Orn(N.delta.-propionyl) residue, the resulting antagonist (BMS-200661) was suitable for use in radioligand binding assays (Kd = 10-30 nM). Antagonist activity obsd. for selected compds. was verified through secondary assays in that these analogs prevented SFLLRNP-NH2-stimulated GTPase activity in platelet membranes and Ca2+ mobilization in cultured human smooth muscle cells and mouse fibroblasts. Furthermore, this inhibition occurred at concns. that had no effect on thrombin catalytic activity, indicating a specific activity attributable to receptor binding and not enzyme inhibition.

CC 1-3 (Pharmacology)
Section cross-reference(s): 34

ST thrombin receptor agonist antagonist peptide

IT Thrombin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(agonists; development of potent thrombin receptor agonist and antagonist peptides)

IT Thrombin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists; development of potent thrombin receptor agonist and antagonist peptides)
IT Structure-activity relationship
(thrombin receptor agonist; development of potent thrombin receptor agonist and antagonist peptides)
IT Structure-activity relationship
(thrombin receptor antagonist; development of potent thrombin receptor agonist and antagonist peptides)
IT 141923-41-3P 145230-35-9P 145230-42-8P 145230-44-0P
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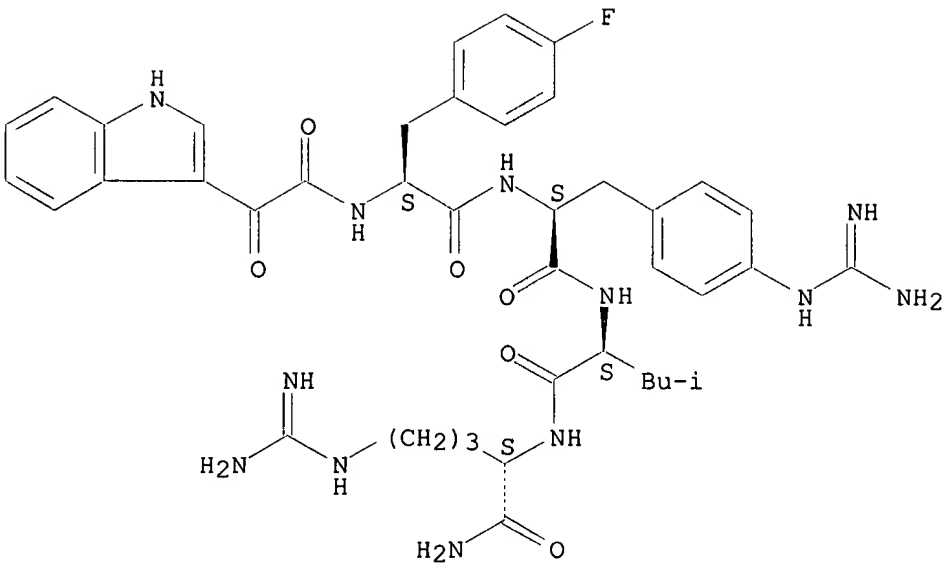
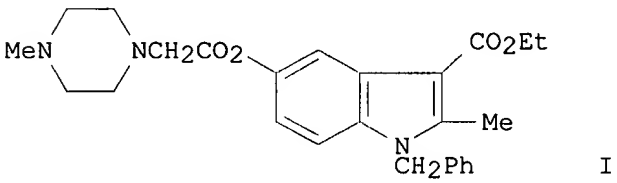
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(development of potent thrombin receptor agonist and antagonist peptides)
IT 9002-04-4, Thrombin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(development of potent thrombin receptor agonist and antagonist peptides)
IT **185028-01-7P**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(development of potent thrombin receptor agonist and antagonist peptides)
RN 185028-01-7 HCAPLUS
CN L-Argininamide, 4-fluoro-N-(1H-indol-3-yloxoacetyl)-L-phenylalanyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1995:772256 Document No. 123:339614 Synthesis and antiserotonin activity of ethyl 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles. Purohit, M. G.; Badiger, G. R.; Kalaskar, N. J. (Dep. Chem., Gulbarga Univ., Gulbarga, 585 106, India). Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem., 34B(9), 796-801 (English) 1995. CODEN: IJSBDB. ISSN: 0376-4699. OTHER SOURCES: CASREACT 123:339614.

GI



I

AB Ethyl-5-O-chloroacetyl-2-methylindole-3-carboxylates (2a-e) have been synthesized by the reaction of Et 5-hydroxy-2-methylindole-3-carboxylates (1a-e) with chloroacetyl chloride in dry benzene contg. triethylamine. These indoles (2a-e) on condensation with methylpiperazine in dry acetone in the presence of anhyd. K2CO3, afford Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates (3a-e). Compds. 3a-e are converted into their oxalate derivs. (4a-e). Indole-3-glyoxylyl chlorides (6a-3) have been prepd. from appropriate indoles (5a-e) by reaction with oxalyl chloride in dry ether. These derivs. on condensation with methylpiperazine yield 3-(4-methyl-1-piperazinylglyoxylyl)indoles (7a-e) which are converted into oxalate salts (8a-e). Compds. 4a-e and 8a-e have been screened for their antiserotonin activity. Only compd. 4d (I.HO2CCO2H) is found to exhibit antiserotonin activity.

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28

ST ethyl methylpiperazinylacetylmethylindolecarboxylate antiserotonin activity; methylpiperazinylglyoxylylindole antiserotonin activity

IT Receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(serotoninergic, prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

IT 170884-60-3P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

IT 50-67-9, Serotonin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

IT 79-04-9, Chloroacetyl chloride 79-37-8, Oxalyl chloride 95-20-5
109-01-3, N-Methylpiperazine 120-72-9, 1H-Indole, reactions
144-62-7, Ethanedioic acid, reactions 948-65-2 4560-08-1
5492-71-7 7598-91-6 13228-36-9 22980-09-2 22980-10-5
23746-76-1 50331-29-8 63746-08-7 69496-82-8 170884-51-2
170884-52-3 170884-53-4 170884-55-6 170884-57-8 170884-59-0
170884-61-4 170884-64-7 170884-66-9 170884-68-1 170884-70-5
170884-72-7 170884-73-8 170884-74-9 170884-75-0 170884-76-1
RL: RCT (Reactant)
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

IT 50995-67-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

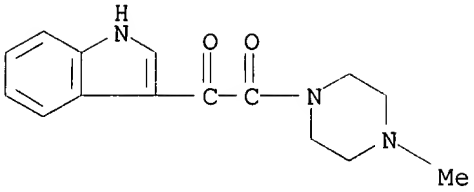
IT 170884-54-5P 170884-56-7P 170884-58-9P 170884-62-5P
170884-63-6P 170884-65-8P 170884-67-0P
170884-69-2P 170884-71-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

IT **170884-63-6P 170884-65-8P 170884-67-0P**
170884-69-2P 170884-71-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and antiserotonin activity of Et 5-O-(4-methylpiperazin-1-ylacetyl)-2-methylindole-3-carboxylates and 3-(4-methyl-1-piperazinylglyoxylyl)indoles)

RN 170884-63-6 HCAPLUS
CN Piperazine, 1-(1H-indol-3-yloxoacetyl)-4-methyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

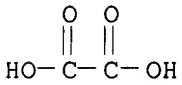
CM 1

CRN 69496-82-8
CMF C15 H17 N3 O2



CM 2

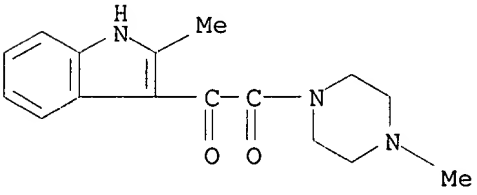
CRN 144-62-7
CMF C2 H2 O4



RN 170884-65-8 HCAPLUS
CN Piperazine, 1-methyl-4-[(2-methyl-1H-indol-3-yl)oxoacetyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

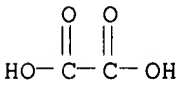
CM 1

CRN 170884-64-7
CMF C16 H19 N3 O2



CM 2

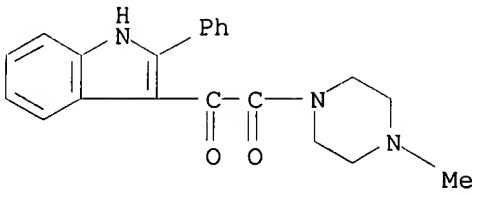
CRN 144-62-7
CMF C2 H2 O4



RN 170884-67-0 HCAPLUS
CN Piperazine, 1-methyl-4-[oxo(2-phenyl-1H-indol-3-yl)acetyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

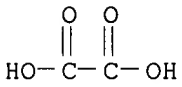
CM 1

CRN 170884-66-9
CMF C21 H21 N3 O2



CM 2

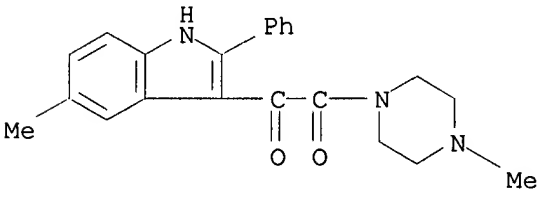
CRN 144-62-7
CMF C2 H2 O4



RN 170884-69-2 HCAPLUS
CN Piperazine, 1-methyl-4-[(5-methyl-2-phenyl-1H-indol-3-yl)oxoacetyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

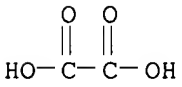
CM 1

CRN 170884-68-1
CMF C22 H23 N3 O2



CM 2

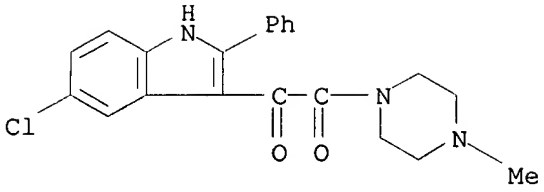
CRN 144-62-7
CMF C2 H2 O4



RN 170884-71-6 HCAPLUS
CN Piperazine, 1-[(5-chloro-2-phenyl-1H-indol-3-yl)oxoacetyl]-4-methyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

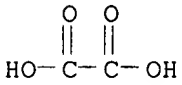
CM 1

CRN 170884-70-5
CMF C21 H20 Cl N3 O2

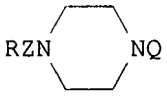


CM 2

CRN 144-62-7
CMF C2 H2 O4



L24 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1995:507921 Document No. 123:55919 Preparation of piperazine derivatives as calmodulin inhibitors. Yamamoto, Kenjiro; Hasegawa, Atsushi; Kubota, Hideki; Ando, Masahiro; Yamaguchi, Hitoshi C. O. Daiichi (Daiichi Pharmaceutical Co. Ltd., Japan). Eur. Pat. Appl. EP 624584 A1 941117, 70 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 94-107496 940513. PRIORITY: JP 93-112771 930514.
GI



I

AB Title compds. I (Q = aryl, heterocyclyl, diarylmethyl, aralkyl composed of an aryl and an alkylene having C1-6, C1-8 alkyl, C3-8 cycloalkyl, in which the aryl, heterocyclyl, and the aryl moiety of the diarylmethyl and aralkyl may be substituted, etc.; R = bicyclic N-contg. heterocyclyl,(substituted)Ph, etc.; Z = C1-3 alkylene, C2-4 alkenylene, HO-C1-3 alkylene, CO, etc.) or salt thereof, are prepd. I R = 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)-1H-indazol-3-yl, Z = CH2CO, Q = 2,3-ClMeC6H3 (prepn. given) in THF and borane-THF complex were refluxed for 2 h to give I (R = 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)-1H-indazol-3-yl, Z = CH2CH2, Q = 2,3-ClMeC6H3). Calmodulin inhibitory activity was demonstrated.
IC ICM C07D403-08
ICS A61K031-495; C07D403-14; C07D405-14; C07D413-14; C07D241-04; C07D405-10; C07D409-10
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST piperrazine analog prepn calmodulin inhibition
IT Calmodulins
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(prepn. of piperazine derivs. as calmodulin inhibitors.)
IT 1245-28-9P 160521-93-7P 160521-99-3P 160522-00-9P

162477-42-1P 162477-43-2P 162495-30-9P 162495-31-0P
162495-32-1P 162495-33-2P 162495-34-3P 162495-35-4P
162495-36-5P 162495-37-6P 162495-38-7P 162495-39-8P
162495-40-1P 162495-41-2P 162495-42-3P 162495-43-4P
162495-44-5P 162495-45-6P 162495-46-7P 162495-47-8P
162495-48-9P 162495-49-0P 162495-50-3P 162495-51-4P
162495-52-5P 162495-53-6P 162495-54-7P 162495-55-8P
162495-56-9P 162495-57-0P 162495-58-1P 162495-59-2P
162495-60-5P 162495-61-6P 162495-62-7P 162495-63-8P
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162495-76-3P 162495-77-4P 162495-78-5P 162495-79-6P
162495-80-9P 162495-81-0P 162495-82-1P 162495-83-2P
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162495-96-7P 162495-97-8P 162495-98-9P 162495-99-0P
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162496-04-0P 162496-05-1P 162496-06-2P 162496-07-3P
162496-08-4P 162496-09-5P 162496-10-8P 162496-11-9P
162496-12-0P 162496-13-1P 162496-14-2P 162496-15-3P
162496-16-4P 162496-17-5P 162496-18-6P 162496-19-7P
162496-20-0P 162496-22-2P 162496-23-3P 162496-24-4P
162496-25-5P 162496-26-6P 162496-27-7P 162496-28-8P
162496-29-9P 162496-30-2P 162496-31-3P 162496-32-4P
162496-33-5P 162496-34-6P 162496-35-7P 162496-36-8P
162496-37-9P 162496-38-0P 162496-39-1P 162496-40-4P
162496-41-5P 162496-42-6P 162496-43-7P 162496-44-8P
162496-45-9P 162496-71-1P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of piperazine derivs. as calmodulin inhibitors.)

IT 93-07-2, Veratric acid 93-17-4, (3,4-Dimethoxyphenyl)acetonitrile 109-06-8, 2-Picoline 120-20-7, 3,4-Dimethoxyphenethylamine 124-68-5, 2-Amino-2-methyl-1-propanol 1822-51-1, 4-(Chloromethyl)pyridine hydrochloride 4302-52-7, (3,4-Dimethoxyphenyl)acetylene 4635-59-0, 4-Chlorobutyryl chloride 6315-89-5, 3,4-Dimethoxyaniline 7306-46-9, 3,4-Dimethoxybenzyl chloride 10313-60-7, 3,4-Dimethoxyphenylacetyl chloride 14430-23-0, 5,6-Dimethoxyindole 18066-68-7, Ethyl (3,4-dimethoxyphenyl)acetate 29281-06-9 35386-24-4 40255-48-9, 1-(2-Aminoethyl)-4-(2-methoxyphenyl)piperazine 50855-25-9, Trimethoxybenzoic acid 54711-70-5, (3-Chloro-2-methylphenyl)piperazine 73357-18-3, (4,5-Dimethoxy-2-nitrophenyl)acetic acid 98224-26-1, 1-(7-Benzofuranyl)piperazine 103057-10-9, 4-(Chloromethyl)1-tritylimidazole 162496-72-2 162496-73-3 162496-75-5 162496-76-6 162496-77-7 162496-78-8, 4-(3-Amino-2-methylphenyl)-1-(benzyloxycarbonyl)piperazine 162496-79-9 162496-80-2
RL: RCT (Reactant)
(prepn. of piperazine derivs. as calmodulin inhibitors.)

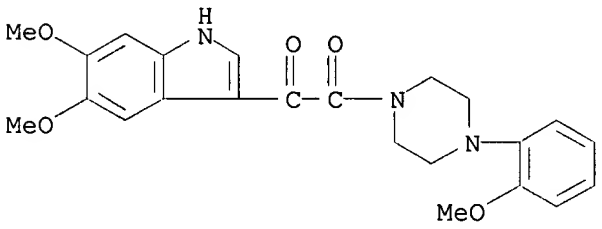
IT 531-88-4P 577-68-4P 4293-90-7P 4821-94-7P 5884-22-0P 14335-78-5P 55159-62-1P 64957-88-6P 68438-33-5P **95442-02-7P** 98205-73-3P 160521-87-9P 160521-88-0P 160521-89-1P 160521-90-4P 160521-91-5P 160521-96-0P 160521-97-1P 160521-98-2P 162137-27-1P 162137-44-2P 162496-46-0P 162496-47-1P 162496-48-2P 162496-49-3P 162496-50-6P 162496-51-7P 162496-52-8P 162496-53-9P 162496-54-0P 162496-55-1P 162496-56-2P 162496-57-3P 162496-58-4P 162496-59-5P 162496-60-8P 162496-61-9P 162496-62-0P 162496-63-1P 162496-64-2P 162496-65-3P 162496-66-4P 162496-67-5P 162496-68-6P 162496-69-7P 162496-70-0P

162496-74-4P 164642-22-2P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of piperazine derivs. as calmodulin inhibitors.)

IT **95442-02-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of piperazine derivs. as calmodulin inhibitors.)

RN 95442-02-7 HCAPLUS

CN Piperazine, 1-[(5,6-dimethoxy-1H-indol-3-yl)oxoacetyl]-4-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



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1994:182348 Document No. 120:182348 Synthesis and benzodiazepine receptor affinity of N-(indol-3-ylglyoxylyl)-dipeptide derivatives. Structural requirements for inverse agonist/antagonist receptor interactions. Da Settimo, Antonio; Primofiore, Giampaolo; Da settimo, Federico; Bianucci, Annamaria; Martini, Claudia; Senatore, Generoso; Lucacchini, Antonio (Ist. Chim. Farm., Univ. Pisa, Pisa, 56126, Italy). Drug Des. Discovery, 10(3), 199-211 (English) 1993. CODEN: DDDIEV. ISSN: 1055-9612.

AB Several N-(indol-3-ylglyoxylyl)dipeptide derivs. were synthesized and tested for their affinity at the benzodiazepine receptor in bovine cortical membranes. They proved to bind with low or no affinity at the receptor site. It was hypothesized that this result was not due to the steric hindrance of the dipeptide side chain, but to the establishment of intramol. hydrogen bonds involving the indole N-H and/or the glyoxylyl (C=O)2. Conformational anal. indicated that coiled conformations, with intramol. hydrogen bonds, were energetically more favored than the staggered, completely unfolded ones. Therefore, the low or no affinity of these compds. should be attributed to the unavailability of the N-H and/or (C=O)2 groups for the binding, again confirming that both of these groups are necessary for interaction with the receptor.

CC 1-3 (Pharmacology)
Section cross-reference(s): 27

ST indolylglyoxylyl dipeptide prepn benzodiazepine receptor affinity

IT Conformation and Conformers
(of indolylglyoxylyl dipeptides, benzodiazepine receptor affinity in relation to)

IT Receptors
RL: BIOL (Biological study)
(benzodiazepine, indolylglyoxylyl dipeptides affinity for, structure in relation to)

IT Molecular structure-biological activity relationship
(benzodiazepine receptor-binding, of indolylglyoxylyl dipeptides)

IT **153694-18-9P 153694-19-0P 153694-20-3P**
153694-21-4P 153694-22-5P 153694-23-6P
153694-24-7P 153694-25-8P 153694-26-9P
153694-27-0P 153694-28-1P 153694-29-2P
RL: **SPN (Synthetic preparation); PREP**

(Preparation)
(prepn. and benzodiazepine receptor affinity of, structure in relation to)

IT 94732-37-3 94732-43-1 97500-73-7 97500-79-3
RL: RCT (Reactant)
(reaction of, with alanine Et ester)

IT 883-55-6 6953-35-1 22980-09-2 63843-81-2
RL: RCT (Reactant)
(reaction of, with dipeptide Et ester)

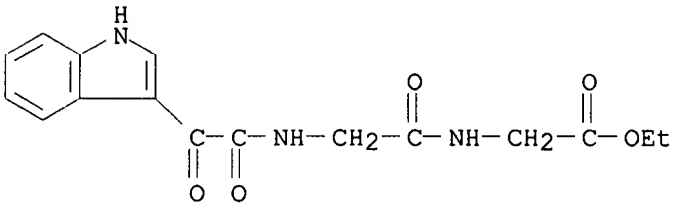
IT 2087-41-4 84794-54-7
RL: RCT (Reactant)
(reaction of, with indolylglyoxylyl chloride)

IT 1115-59-9, Alanine ethyl ester hydrochloride
RL: RCT (Reactant)
(reaction of, with indolylglyoxylylglycine)

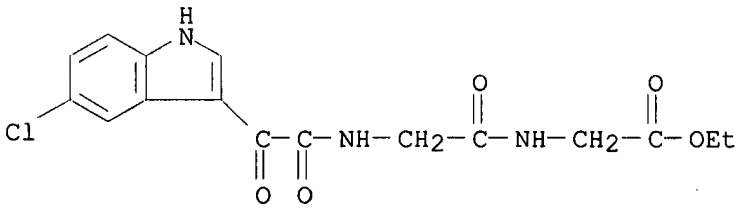
IT 12794-10-4, Benzodiazepine
RL: BIOL (Biological study)
(receptors for, indolylglyoxylyl dipeptides affinity for, structure in relation to)

IT **153694-18-9P 153694-19-0P 153694-20-3P**
153694-21-4P 153694-22-5P 153694-23-6P
153694-24-7P 153694-25-8P 153694-26-9P
153694-27-0P 153694-28-1P 153694-29-2P
RL: **SPN (Synthetic preparation); PREP**
(Preparation)
(prepn. and benzodiazepine receptor affinity of, structure in relation to)

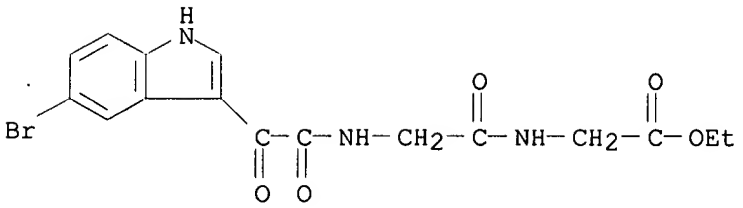
RN 153694-18-9 HCAPLUS
CN Glycine, N-[[(1H-indol-3-yloxoacetyl)amino]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



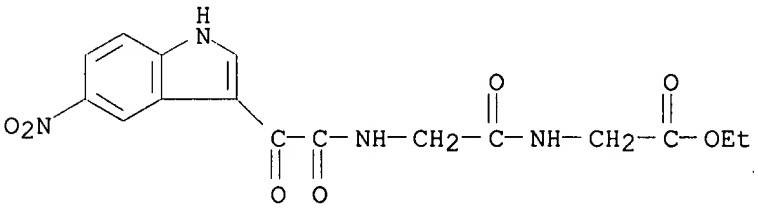
RN 153694-19-0 HCAPLUS
CN Glycine, N-[[[(5-chloro-1H-indol-3-yl)oxoacetyl]amino]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 153694-20-3 HCAPLUS
CN Glycine, N-[[[(5-bromo-1H-indol-3-yl)oxoacetyl]amino]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

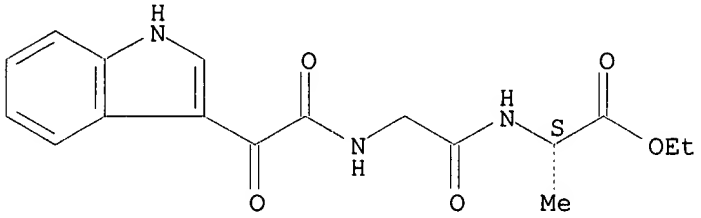


RN 153694-21-4 HCAPLUS
CN Glycine, N-[[[(5-nitro-1H-indol-3-yl)oxoacetyl]amino]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



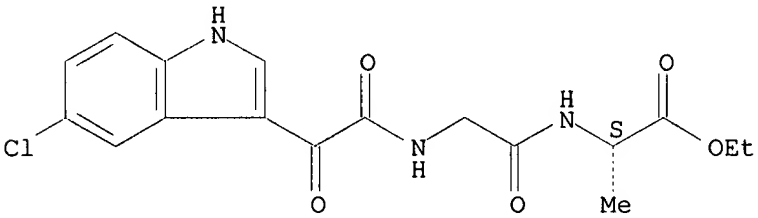
RN 153694-22-5 HCAPLUS
CN L-Alanine, N-[N-(1H-indol-3-yloxoacetyl)glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



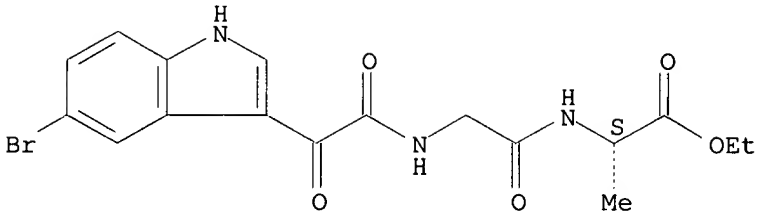
RN 153694-23-6 HCAPLUS
CN L-Alanine, N-[N-[(5-chloro-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



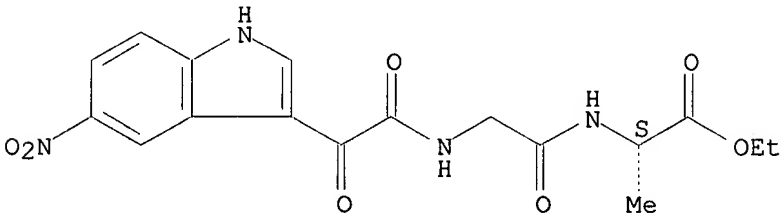
RN 153694-24-7 HCAPLUS
CN L-Alanine, N-[N-[(5-bromo-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



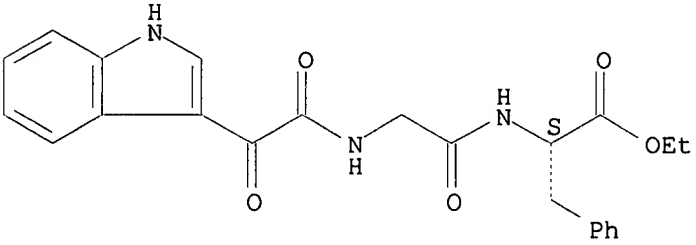
RN 153694-25-8 HCAPLUS
CN L-Alanine, N-[N-[(5-nitro-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



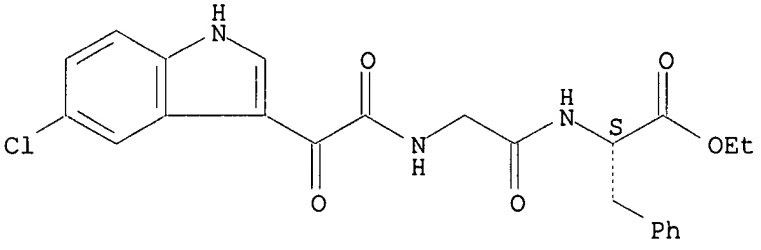
RN 153694-26-9 HCAPLUS
CN L-Phenylalanine, N-[N-(1H-indol-3-yloxoacetyl)glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



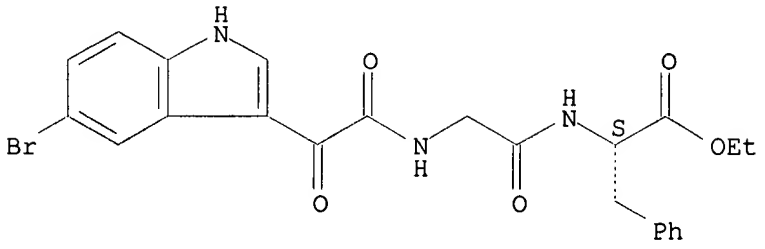
RN 153694-27-0 HCAPLUS
CN L-Phenylalanine, N-[N-[(5-chloro-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



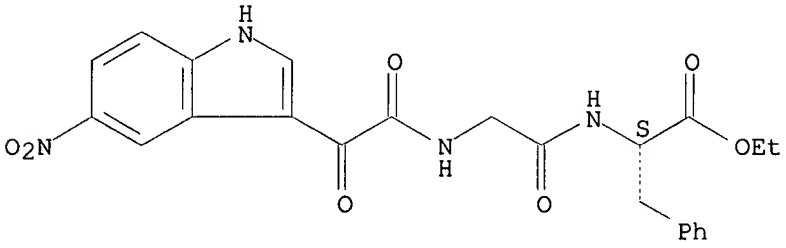
RN 153694-28-1 HCAPLUS
CN L-Phenylalanine, N-[N-[(5-bromo-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

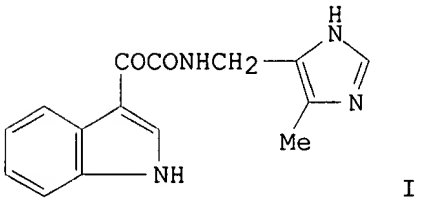


RN 153694-29-2 HCAPLUS
CN L-Phenylalanine, N-[N-[(5-nitro-1H-indol-3-yl)oxoacetyl]glycyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



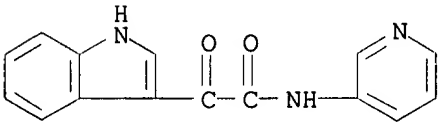
L24 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1994:125105 Document No. 120:125105 Probing the 5-HT3 receptor site using novel indole-3-glyoxylic acid derivatives. Evans, S. M.; Huang, B. S.; Feng, D.; Gall, M.; Tsai, C.; Bariso, C.; Taylor, C. A. (ABOC Health Care Co., Anaquest Inc., Murray Hill, NJ, 07974, USA). Med. Chem. Res., 3(5-6), 386-406 (English) 1993. CODEN: MCREEB. ISSN: 1054-2523.
GI



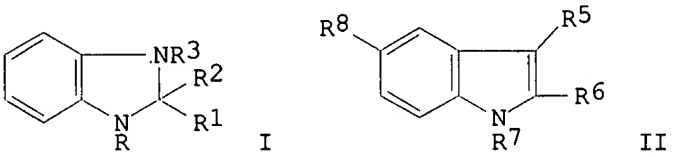
I

AB Novel ester and amide derivs. of indole-3-glyoxylic acid were synthesized and used to probe the 5-HT3 receptor binding site. The structural design of these ligands was based on 1) the rigidity and preferred conformation of the glyoxylic acid fragment, as shown by ab initio geometry optimization using the 3-21G basis set, and 2) the chem. template comprising the 3-dimensional pharmacophore for the 5-HT3 recognition site. The geometrical changes provide ligands which are selective for the 5-HT3 receptor and demonstrate good antiemetic potency. The most potent compd. (I) had a binding affinity of 33 nM and an ED50 of 0.07 mg/kg i.v. in the

cisplatin-induced emesis assay in ferrets.
CC 2-2 (Mammalian Hormones)
ST serotoninergic S3 receptor ligand; indoleglyoxylate deriv serotonin receptor
IT Pharmacophores
(of serotoninergic S3 receptors)
IT Receptors
RL: BIOL (Biological study)
(serotoninergic S3, indoleglyoxylate derivs. as ligands for)
IT 132797-95-6P 143137-38-6P 152721-50-1P 152721-51-2P
152721-52-3P 152721-53-4P 152721-54-5P 152721-55-6P
152721-56-7P **152721-57-8P** 152721-58-9P 152721-59-0P
152721-60-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and serotoninergic S3 receptor binding of)
IT 51605-33-5P, 4-Chloromethyl-5-methylimidazole hydrochloride
72631-77-7P 152721-61-4P 152721-62-5P 152721-63-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **152721-57-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and serotoninergic S3 receptor binding of)
RN 152721-57-8 HCAPLUS
CN 1H-Indole-3-acetamide, .alpha.-oxo-N-3-pyridinyl- (9CI) (CA INDEX NAME)

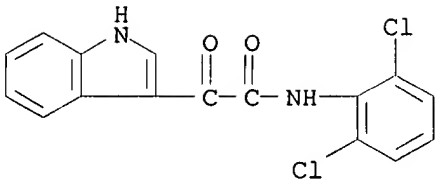


L24 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1991:449510 Document No. 115:49510 Synthesis and antihypertensive activity of some 2-aminobenzimidazole and indole derivatives. Da Settimo, Antonio; Marini, Anna Maria; Primofiore, Giampaolo; Subissi, Alessandro (Ist. Chim. Farm., Univ. Pisa, Pisa, 56100, Italy). Farmaco, 46(2), 357-67 (English) 1991. CODEN: FRMCE8.
GI

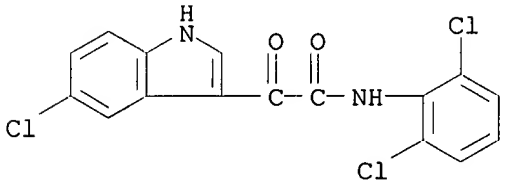


AB Aminobenzimidazole derivs. I [R = H, CH2Ph, Me, CH2C6H4Cl-4, R1 = NHCOCOR4, R2R3 = bond, R4 = 2,6-dichloroanilino (throughout); R = H, CH2Ph, Me, CH2C6H4Cl-4, R1R2 = NH, R3 = CH2COR4] and indole derivs. II (R5 = COCOR4, R6,R7 = H, Me, R8 = H, Br, Cl, NO2, OMe; R5 = CH2COR4, R6 = R7 = R8 = H) were prepd. and some were tested for antihypertensive activity. Thus, indol-3-ylacetyl chloride condensed with 2,6-dichloroaniline to give II (R5 = CH2COR4, R6 = R7 = R8 = H). None of the compds. tested showed appreciable antihypertensive activity.

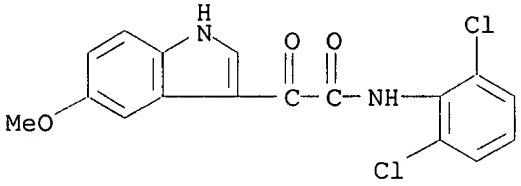
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST aminobenzimidazole prepn antihypertensive; benzimidazole amino prepn antihypertensive; indole prepn antihypertensive; antihypertensive aminobenzimidazole indole
IT Antihypertensives
(aminobenzimidazole and indole derivs., inactive)
IT 95-20-5, 2-Methylindole 120-72-9, Indole, reactions 875-79-6, 1,2-Dimethylindole 934-32-7, 2-Aminobenzimidazole 1006-94-6, 5-Methoxyindole 1622-57-7, 2-Amino-1-methylbenzimidazole 6146-52-7, 5-Nitroindole 10075-50-0, 5-Bromoindole 17422-32-1, 5-Chloroindole 43182-10-1, 2-Amino-1-benzylbenzimidazole 109635-38-3
RL: RCT (Reactant)
(acylation of, with oxalyl chloride)
IT 3644-56-2
RL: RCT (Reactant)
(alkylation by, of benzimidazole derivs. and theophylline)
IT 58-55-9, Theophylline, reactions
RL: RCT (Reactant)
(alkylation of, with (dichlorphenyl)chloroacetamide)
IT 50720-05-3, Indol-3-ylacetyl chloride
RL: RCT (Reactant)
(amidation of, by dichloroaniline)
IT 608-31-1, 2,6-Dichloroaniline
RL: RCT (Reactant)
(amination by, of benzimidazole and indole derivs.)
IT 26893-41-4P 110179-22-1P 116008-63-0P 134937-64-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of, with oxalyl chloride)
IT 883-55-6P 2426-19-9P 6953-35-1P 22980-09-2P 22980-10-5P 63843-81-2P 117196-94-8P 134937-65-8P 134937-66-9P 134937-67-0P 134937-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amination of, with dichloroaniline)
IT 134937-70-5P 134937-72-7P 134937-73-8P 134937-74-9P 134937-80-7P **134937-81-8P 134937-83-0P 134937-85-2P 134937-87-4P** 134937-88-5P 134937-89-6P
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(prepn. and antihypertensive activity of)
IT 134937-69-2P 134937-71-6P 134937-75-0P 134937-76-1P 134937-77-2P 134937-78-3P 134937-79-4P **134937-82-9P 134937-84-1P 134937-86-3P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(prepn. of)
IT **134937-81-8P 134937-83-0P 134937-85-2P 134937-87-4P**
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(prepn. and antihypertensive activity of)
RN 134937-81-8 HCAPLUS
CN 1H-Indole-3-acetamide, N-(2,6-dichlorophenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



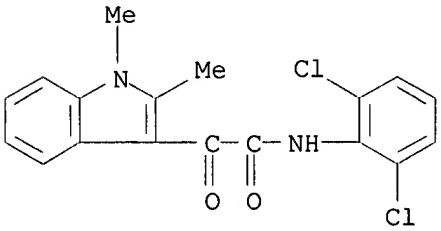
RN 134937-83-0 HCAPLUS
CN 1H-Indole-3-acetamide, 5-chloro-N-(2,6-dichlorophenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



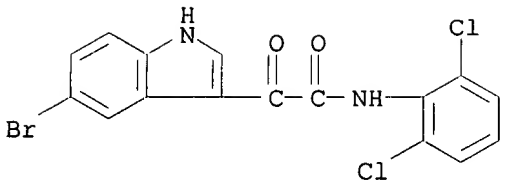
RN 134937-85-2 HCAPLUS
CN 1H-Indole-3-acetamide, N-(2,6-dichlorophenyl)-5-methoxy-.alpha.-oxo- (9CI) (CA INDEX NAME)



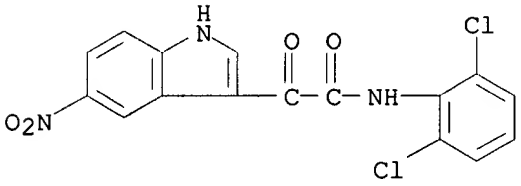
RN 134937-87-4 HCAPLUS
CN 1H-Indole-3-acetamide, N-(2,6-dichlorophenyl)-1,2-dimethyl-.alpha.-oxo- (9CI) (CA INDEX NAME)



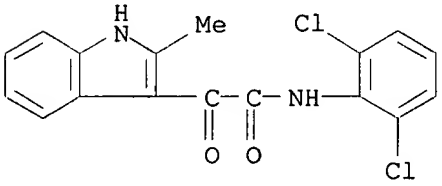
IT **134937-82-9P 134937-84-1P 134937-86-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
RN 134937-82-9 HCAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N-(2,6-dichlorophenyl)-.alpha.-oxo- (9CI) (CA INDEX NAME)



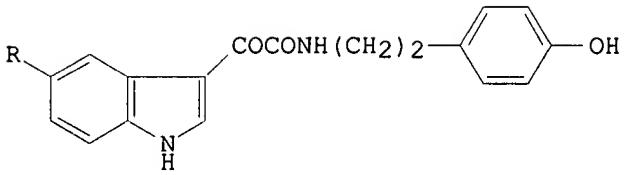
RN 134937-84-1 HCAPLUS
CN 1H-Indole-3-acetamide, N-(2,6-dichlorophenyl)-5-nitro-.alpha.-oxo- (9CI) (CA INDEX NAME)



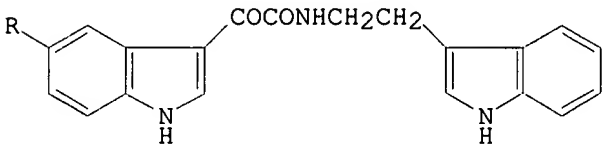
RN 134937-86-3 HCAPLUS
CN 1H-Indole-3-acetamide, N-(2,6-dichlorophenyl)-2-methyl-.alpha.-oxo- (9CI) (CA INDEX NAME)



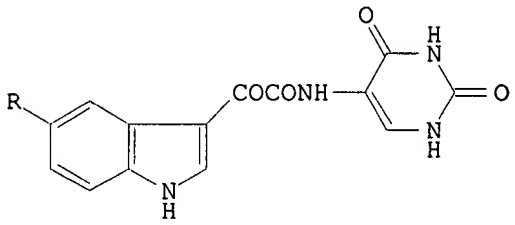
L24 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1987:432773 Document No. 107:32773 Synthesis and anti-inflammatory activity of some N-(5-substituted indol-3-ylglyoxyl)amine derivatives. Da Settimo, A.; Primofiore, G.; Marini, A. M.; Mori, C.; Franzone, J. S.; Cirillo, R.; Reboani, C. (Ist. Chim. Farm., Univ. Pisa, Pisa, Italy). Farmaco, Ed. Sci., 42(1), 17-26 (English) 1987. CODEN: FRPSAX. ISSN: 0430-0920.
GI



I



II



III

AB The title compds. [e.g. I; II; and III; R = H, Cl, Br, NO2, or OMe] were prepd. by condensation of the various 5-substituted indolylglyoxal chlorides with the resp. amines. The prepd. compds. showed only weak anti-inflammatory and analgesic activity by various tests in mice or rats.

CC 1-7 (Pharmacology)
Section cross-reference(s): 27, 28

ST indolylglyoxylamine prepn analgesic antiinflammatory

IT Analgesics
Inflammation inhibitors
((indolglyoxyl)amine derivs., prepn. of)

IT 60-19-5 343-94-2 932-52-5, 5-Aminouracil
RL: RCT (Reactant)
(condensation reaction of, with indolylglyoxyl chlorides)

IT 883-55-6 2426-19-9 6953-35-1
RL: RCT (Reactant)
(condensation reaction of, with tyramine and tryptaomine hydrochloride)

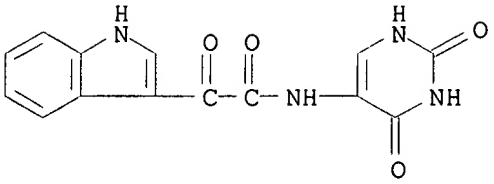
IT 107610-00-4P 107610-01-5P 107610-02-6P 107610-03-7P
107610-04-8P 107610-05-9P 107610-06-0P 107610-07-1P
107610-08-2P 107610-09-3P 107610-10-6P
107610-11-7P 107610-12-8P 107610-13-9P 107634-84-4P
107634-85-5P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and anti-inflammatory and analgesic activity of)

IT 22980-09-2 63843-81-2
RL: RCT (Reactant)
(reaction of, with tyramine and tryptamine hydrochloride and aminouracil)

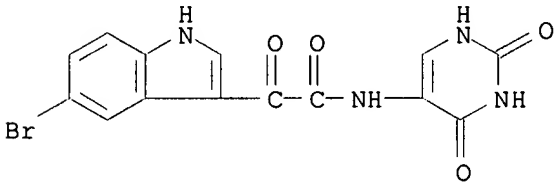
IT **107610-08-2P 107610-09-3P 107610-10-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and anti-inflammatory and analgesic activity of)

RN 107610-08-2 HCAPLUS

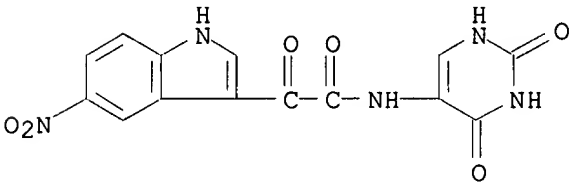
CN 1H-Indole-3-acetamide, .alpha.-oxo-N-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



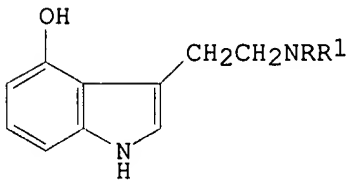
RN 107610-09-3 HCAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-.alpha.-oxo-N-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 107610-10-6 HCAPLUS
CN 1H-Indole-3-acetamide, 5-nitro-.alpha.-oxo-N-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1981:461908 Document No. 95:61908 Psilocin analogs. II. Synthesis of 3-[2-(dialkylamino)ethyl]-, 3-[2-(N-methyl-N-alkylamino)ethyl]-, and 3-[2-(cycloalkylamino)ethyl]indol-4-ols. Repke, David B.; Ferguson, Wilfred J.; Bates, Dallas K. (Los Altos, CA, 94022, USA). J. Heterocycl. Chem., 18, 175-9 (English) 1981. CODEN: JHTCAD. ISSN: 0022-152X.
GI



I

AB Psilocin analogs I (R, R1 = Me2CHCH2, MeCH2CHMe, Me, Et, Pr, Me2CH, Bu, cyclopentyl; NRR1 = substituted piperidyl, piperazino) were prepd. by condensation of 4-acetoxyindole with ClCOCOCl and HNRR1, followed by LiAlH4 redn.
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

ST psilocin analog; acetoxyindole condensation oxalyl chloride amine; aminoethylindolol; indole hydroxyaminoethyl; hydroxyindole aminoethyl; hydroxytryptamine

IT Psychotropics
(psilocin analog)

IT 1190-92-7
RL: RCT (Reactant)
(condensation of, with acetoxyindole)

IT 5585-96-6
RL: RCT (Reactant)
(condensation of, with oxalyl chloride and amines)

IT 77872-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and attempted redn. of)

IT 30000-66-9P 77872-23-2P 77872-24-3P 77872-25-4P 77872-26-5P
77872-27-6P 77872-28-7P 77872-29-8P 77872-30-1P 77872-31-2P
77872-32-3P 77872-33-4P 77872-34-5P 77872-35-6P 77872-36-7P
77872-37-8P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)

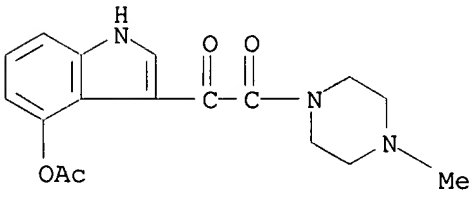
IT 520-53-6P 59044-64-3P 77872-38-9P 77872-39-0P 77872-40-3P
77872-41-4P 77872-42-5P 77872-43-6P 77872-44-7P 77872-45-8P
77872-46-9P 77872-47-0P 77872-48-1P 77872-49-2P 77872-50-5P
77872-51-6P 77872-53-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 77872-52-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., redn., and acetylation of)

IT **77872-37-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)

RN 77872-37-8 HCAPLUS

CN Piperazine, 1-[[4-(acetyloxy)-1H-indol-3-yl]oxoacetyl]-4-methyl- (9CI) (CA INDEX NAME)

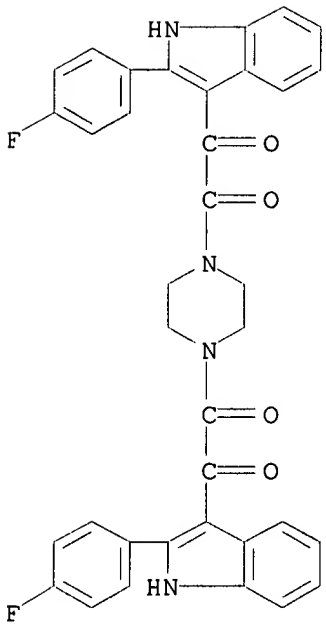


L24 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 1998 ACS

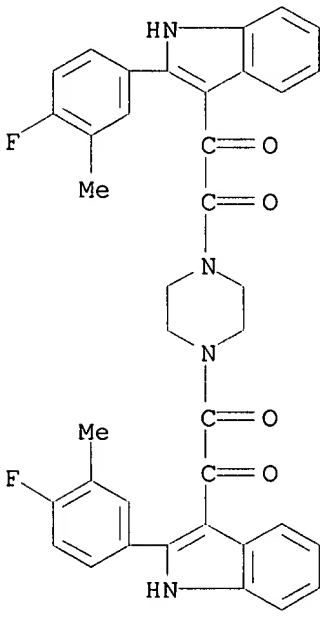
1981:174796 Document No. 94:174796 Synthesis of some new fluorine containing 3-dialkylaminomethyl indoles, 3-indolylglyoxamides and tryptamines. Joshi, Krishna C.; Pathak, Vijai N.; Singh, Raj Pal (Dep. Chem., Univ. Rajasthan, Jaipur, 302004, India). Monatsh. Chem., 111(6), 1343-50 (English) 1980. CODEN: MOCMB7. ISSN: 0026-9247.

AB 3-Acetyl-2-(fluoroaryl)indoles, 2-(fluoroaryl)-3-indolylglyoxamides and the corresponding tryptamines were prepd. as possible psychopharmacol. agents. 2-(Fluoroaryl)indoles were prepd. by the Fischer indole synthesis. Treating 2-(fluoroaryl)indoles with oxalyl chloride and then with amines gave 2-(fluoroaryl)-3-indolylglyoxamides, some of which were reduced by LiAlH4 to give tryptamines. Mannich reaction of 2-(fluoroaryl)indoles gave 3-(dialkylaminoamethyl)-2-(fluoroaryl)indoles.

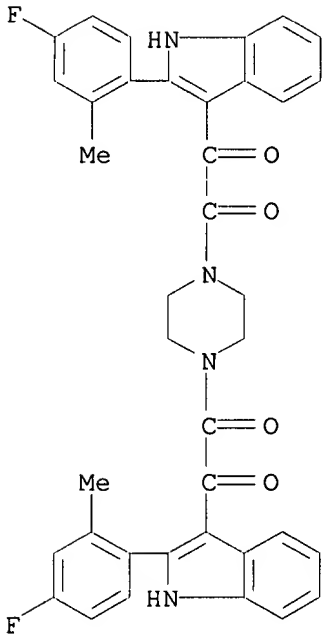
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
ST indole aminomethyl prepn psychopharmacolog; indolylglyoxamide prepn psychopharmacolog; tryptamine prepn psychopharmacolog; central nervous system indole deriv
IT Nervous system
(central, indole derivs., potential effect on)
IT 109-89-7, reactions 110-89-4, reactions 110-91-8, reactions 124-40-3, reactions
RL: RCT (Reactant)
(Mannich reaction of, with aryl indoles)
IT 77445-94-4 77445-95-5 77445-96-6 77445-97-7 77445-98-8 77445-99-9 77446-00-5
RL: RCT (Reactant)
(cyclization of, aryl indoles from)
IT 77445-88-6P 77445-89-7P 77445-90-0P 77445-91-1P 77445-92-2P 77445-93-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amidation of)
IT 77445-45-5P 77445-46-6P 77445-47-7P 77445-48-8P 77445-50-2P 77445-51-3P 77445-54-6P 77445-56-8P 77445-58-0P 77445-59-1P 77445-60-4P 77445-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydride redn. of)
IT 77445-11-5P 77445-12-6P 77445-13-7P 77445-14-8P 77445-15-9P 77445-16-0P 77445-17-1P 77445-18-2P 77445-20-6P 77445-21-7P 77445-22-8P 77445-23-9P 77445-25-1P 77445-26-2P 77445-27-3P 77445-28-4P 77445-29-5P 77445-30-8P 77445-31-9P 77445-32-0P 77445-33-1P 77445-34-2P 77445-35-3P 77445-37-5P 77445-38-6P 77445-39-7P 77445-40-0P 77445-41-1P 77445-42-2P 77445-43-3P 77445-44-4P 77445-49-9P 77445-52-4P 77445-53-5P 77445-55-7P 77445-57-9P 77445-61-5P 77445-62-6P 77445-64-8P 77445-65-9P 77445-66-0P 77445-67-1P 77445-68-2P **77445-69-3P** **77445-70-6P** **77445-71-7P** **77445-72-8P** **77445-73-9P** **77445-74-0P** 77445-75-1P 77445-76-2P 77445-77-3P 77445-78-4P 77445-79-5P 77445-80-8P 77445-81-9P 77445-82-0P 77445-83-1P 77445-84-2P 77445-85-3P 77445-86-4P 77452-94-9P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
IT 347-09-1P 782-17-2P 1868-88-8P 70059-35-7P 70059-36-8P 70059-37-9P 70093-24-2P 77445-08-0P 77445-09-1P 77445-10-4P 77445-87-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., acylation, and Mannich reactions of)
IT **77445-69-3P** **77445-70-6P** **77445-71-7P** **77445-72-8P** **77445-73-9P** **77445-74-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
RN 77445-69-3 HCAPLUS
CN Piperazine, 1,4-bis[[2-(4-fluorophenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)



RN 77445-70-6 HCAPLUS
CN Piperazine, 1,4-bis[[2-(4-fluoro-3-methylphenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)

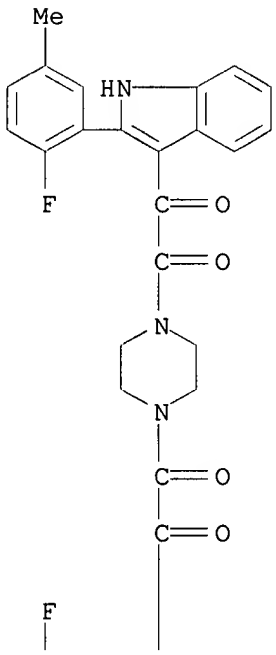


RN 77445-71-7 HCAPLUS
CN Piperazine, 1,4-bis[[2-(4-fluoro-2-methylphenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)

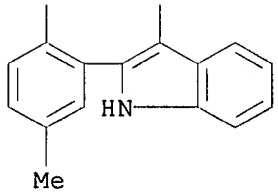


RN 77445-72-8 HCAPLUS
CN Piperazine, 1,4-bis[[2-(2-fluoro-5-methylphenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

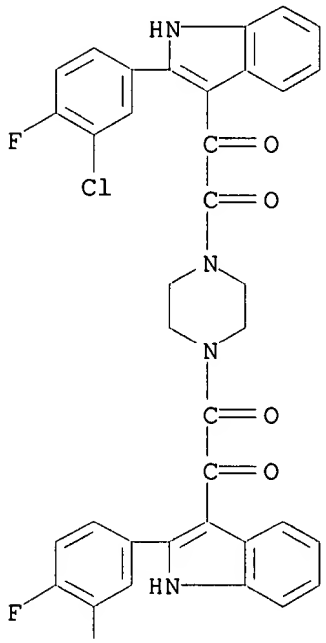


PAGE 2-A



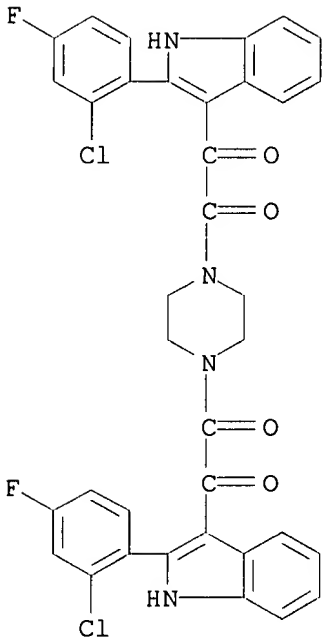
RN 77445-73-9 HCAPLUS
CN Piperazine, 1,4-bis[[2-(3-chloro-4-fluorophenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



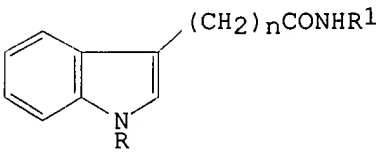
PAGE 2-A

RN 77445-74-0 HCAPLUS
CN Piperazine, 1,4-bis[[2-(2-chloro-4-fluorophenyl)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)

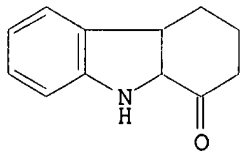


L24 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1980:128647 Document No. 92:128647 Indole derivatives. CXIV. Synthesis of anilides of indolylalkanoic acids. Eryshev, B. Ya.; Ershova, T. D.; Buyanov, V. V.; Suvorov, N. N. (USSR). Tr. - Mosk. Khim.-Tekhnol. Inst. im. D. I. Mendeleeva, 94, 42-5 (Russian) 1977. CODEN: TMKIAT. ISSN: 0371-9723.

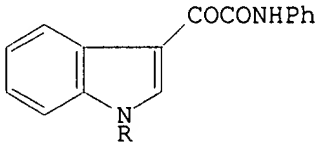
GI



I



II



III

AB Anilides I (R = H, Ac; R1 = Ph, p-ClC6H4, p-O2NC6H4, 3,4-Cl2C6H3; n = 0, 1, 2, 3) were prepd. in 30-95.3% yield. I (R = H; R1 = p-tolyl, benzyl, 3,4-Cl2C6H3; n = 1) were also prepd. in 44-93.7% yield by reaction of the acid or acid chloride with R1NH2. Carbazole II was prepd. in 87% yield by cyclization of .gamma.-3-indolylbutyric acid. Anilides III (R = H, Ac) were prepd. similarly in 80 and 36.8% yield resp. No antiiflammatory activity was detected.

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

ST cyclization indolylbutyrate; anilide indolylalkanoate prepn antiinflammatory

IT 133-32-4

RL: RCT (Reactant)
(cyclization of)

IT 3456-99-3P 57932-47-5P 73031-08-0P 73031-09-1P 73031-10-4P
73031-11-5P 73031-12-6P 73031-13-7P 73031-14-8P 73031-15-9P
73031-16-0P 73031-17-1P 73031-18-2P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

IT 79-37-8
RL: RCT (Reactant)
(reaction of, with acetylindole)

IT 22980-09-2
RL: RCT (Reactant)
(reaction of, with aniline)

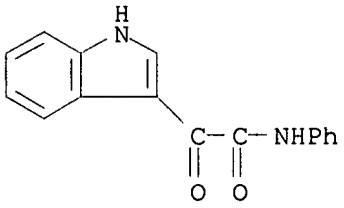
IT 95-76-1 100-46-9, reactions 106-49-0, reactions
RL: RCT (Reactant)
(reaction of, with indolylacetic acid)

IT 53330-94-2
RL: RCT (Reactant)
(reaction of, with oxalyl chloride)

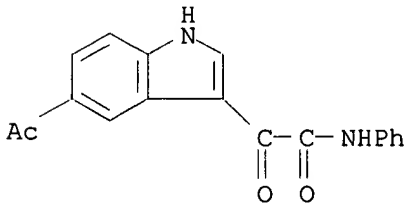
IT 87-51-4, reactions
RL: RCT (Reactant)
(reaction of, with toluidine)

IT **73031-16-0P 73031-17-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 73031-16-0 HCAPLUS
CN 1H-Indole-3-acetamide, .alpha.-oxo-N-phenyl- (9CI) (CA INDEX NAME)

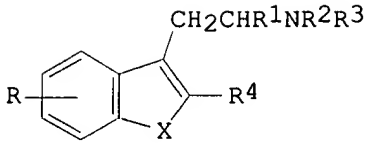


RN 73031-17-1 HCAPLUS
CN 1H-Indole-3-acetamide, 5-acetyl-.alpha.-oxo-N-phenyl- (9CI) (CA INDEX NAME)



L24 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1979:132591 Document No. 90:132591 Serotonin receptor binding affinities of tryptamine analogs. Glennon, Richard A.; Gessner, Peter K. (Med. Coll. Virginia, Virginia Commonwealth Univ., Richmond, Va., USA). J. Med. Chem., 22(4), 428-32 (English) 1979. CODEN: JMCMAR. ISSN: 0022-2623.

GI



I

AB The serotonin (5-HT) [50-67-9] receptor binding affinities of 27 tryptamine analogs I (R = H, OH, OMe, NH2, Ac, etc.; R1 = H, Me, or Et; R2 = H, Me, etc.; R3 = H, Me, Et, etc.; R4 = H or Me; X = NH, NMe, CH2, or S), some of which were prepd., were detd. using a rat fundus model. Bufotenine hydrogen oxalate (I; R = 5-OH, R1 = H, R2 = Me, R3 = Me, R4 = H, and X = NH) [2963-79-3] had the highest apparent affinity for 5-HT receptors. In general, a hydroxy or MeO group at the 5 position greatly enhanced affinity. Replacement of the indolic N by an Sp3 hybridized C atom or moving the MeO group from the 5 position to the 4, 6, or 7 position on the indolic nucleus decreased affinity. Replacing the indolic N by S had no effet on affinity. Affinity decreased as the steric bulk around the terminal amine increased. No direct relationship between affinity and either the pKa values or lipid soly., as reflected by partition coeff., was obsd. for 9 I examd. The relationship between the 5-HT receptor binding affinities and the psychotomimetic potencies of several I is discussed.

CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 27

ST tryptamine analog serotonin receptor binding; psychotomimetic serotonin receptor binding

IT Psychotomimetics
(tryptamine analogs, serotonin receptor binding of, structure in relation to)

IT Molecular structure-biological activity relationship
(serotonin-receptor binding, of tryptamine analogs)

IT Receptors
RL: BIOL (Biological study)
(serotoninergic, tryptamine analogs binding to, structure in relation to)

IT **69496-82-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)

IT 1095-26-7P 69496-78-2P 69496-79-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and serotonin receptor binding of)

IT 4342-14-7P 69496-81-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

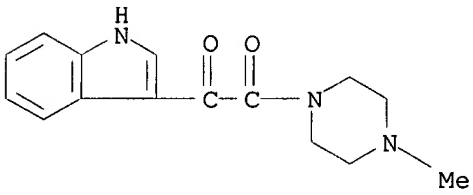
IT 109-01-3
RL: RCT (Reactant)
(reaction of, with indole and oxalyl chloride)

IT 120-72-9, biological studies
RL: RCT (Reactant)
(reaction of, with oxalyl chloride and methylpiperazine)

IT 50-67-9, biological studies
RL: BIOL (Biological study)
(receptor for, tryptamine analogs binding to, structure in relation to)

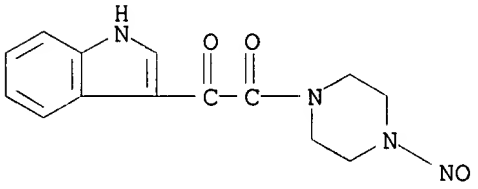
IT 61-50-7 118-68-3 343-94-2 520-53-6 879-36-7 1010-95-3
2454-70-8 2963-79-3 7578-26-9 10438-57-0 13117-35-6
14780-23-5 17286-40-7 19446-09-4 19446-11-8 19446-13-0
20671-78-7 60331-61-5 65487-75-4 65882-40-8 69496-76-0
69496-77-1 69496-80-6 69521-25-1
RL: PROC (Process)

(serotonin receptor binding of)
IT 61-54-1D, analogs
RL: PROC (Process)
(serotonin receptor binding of, structure in relation to)
IT **69496-82-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)
RN 69496-82-8 HCAPLUS
CN Piperazine, 1-(1H-indol-3-yloxoacetyl)-4-methyl- (9CI) (CA INDEX NAME)

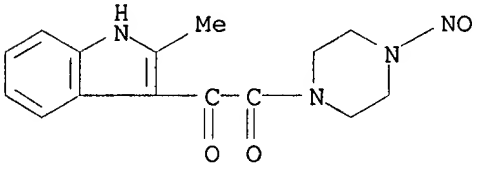


L24 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1977:561423 Document No. 87:161423 Synthesis of 3-(4-acylaminopiperazin-1-ylalkyl)indoles as potential antihypertensive agents. Glamkowski, Edward J.; Reitano, Philip A.; Woodward, David L. (Chem. Res. Dep., Hoechst-Roussel Pharm. Inc., Somerville, N. J., USA). J. Med. Chem., 20(11), 1485-9 (English) 1977. CODEN: JMCMAR.
GI For diagram(s), see printed CA Issue.
AB A series of 31 title compds. was prepd. by acylation of the appropriate indole deriv. with ClCOCOCl, reaction with N-nitrosopiperazine [5632-47-3], redn., and acylation, or from gramine [87-52-5] by reaction with N-nitrosopyerazine, redn., and acylation. In tests in spontaneous hypertensive rats, five compds. lowered blood pressure > 55 mm Hg at oral doses of 100 mg/kg, and I [58433-87-7] was in the potency range of indoramin. Structure-activity relations are discussed.
CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 27, 28
ST antihypertensive acylaminopiperazinylalkylindole deriv
IT Antihypertensives
((acylaminopiperazinylalkyl)indole derivs.)
IT Molecular structure-biological activity relationship
(antihypertensive, of (acylaminopiperazinylalkyl) indole derivs.)
IT 22980-09-2
RL: RCT (Reactant)
(acylation by, of piperazine deriv.)
IT 5632-47-3
RL: RCT (Reactant)
(acylation of)
IT 58433-73-1P 58433-75-3P 58433-77-5P 58434-06-3P 58434-13-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of)
IT 58433-78-6P 58433-79-7P 58433-80-0P 58433-81-1P 58433-82-2P
58433-83-3P 58433-84-4P 58433-87-7P 58433-89-9P 58433-91-3P
58433-92-4P 58433-93-5P 58433-94-6P 58433-95-7P 58433-96-8P
58433-99-1P 58434-00-7P 58434-01-8P 58434-03-0P 58434-04-1P
58434-08-5P 58434-09-6P 58434-10-9P 58434-11-0P 58434-14-3P
58434-15-4P 58434-16-5P 58434-17-6P 58434-18-7P 58434-19-8P
58434-20-1P 64231-15-8P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

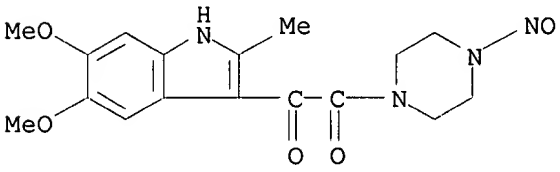
(prepn. and antihypertensive activity of)
IT **58433-72-0P 58433-74-2P** 58433-76-4P
58434-12-1P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)
IT 87-52-5
RL: RCT (Reactant)
(reaction of, with piperazine deriv.)
IT **58433-72-0P 58433-74-2P 58434-12-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)
RN 58433-72-0 HCAPLUS
CN Piperazine, 1-(1H-indol-3-yloxoacetyl)-4-nitroso- (9CI) (CA INDEX NAME)



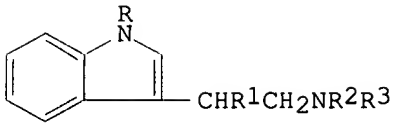
RN 58433-74-2 HCAPLUS
CN Piperazine, 1-[(2-methyl-1H-indol-3-yl)oxoacetyl]-4-nitroso- (9CI) (CA INDEX NAME)



RN 58434-12-1 HCAPLUS
CN Piperazine, 1-[(5,6-dimethoxy-2-methyl-1H-indol-3-yl)oxoacetyl]-4-nitroso- (9CI) (CA INDEX NAME)



L24 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1977:106379 Document No. 86:106379 3-(2-Aminoethyl)indole derivatives. Fernandez Alvarez, Eldiberto; Alemany Soto, Antonio (Spain). Span. ES 421186 760416, 17 pp. (Spanish). CODEN: SPXXAD. APPLICATION: ES 731205.
GI



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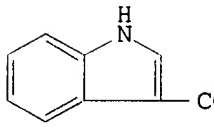


II

AB (Aminoethyl)indoles I (R = H, Me, PhCH2; R1 = H, OH; R2 = H, propargyl; R3 = Me, Et, Me2CH, PhCH2) and their salts were prepd. in several steps from indole or its N-alkyl derivs. Thus, treatment of indole with oxalyl chloride in ether gave II (R4 = Cl), which with MeNH2 gave II (R4 = MeNH). Redn. of the latter with LiAlH4 and then treatment with HC.tplbond.CCH2Br gave I (R = R1 = H, R2 = propargyl, R3 = Me), which was characterized as its HBr and picrate salts. The redn. step in the case of N-alkylated indoleglyoxylamides (R = Me, PhCH2) led to the hydroxy compds. (R1 = OH).

IC C07C

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

ST indole aminoethyl; aminoethylindole

IT 79-37-8
RL: RCT (Reactant)
(acylation by, of indoles)

IT 120-72-9, reactions 603-76-9 3377-71-7
RL: RCT (Reactant)
(acylation of, with oxalyl chloride)

IT 16382-38-0P 22980-09-2P 55654-68-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amidation of)

IT 61-49-4P 61-53-0P 7319-65-5P 7319-69-9P 15741-79-4P
55654-87-0P 55654-91-6P 55654-93-8P 55654-96-1P 62002-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with propargyl bromide)

IT 2054-72-0P 7352-90-1P 55654-69-8P 55654-71-2P 55654-72-3P
55654-73-4P 55654-74-5P 55654-75-6P 55654-76-7P 55654-77-8P
62001-96-1P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)

IT 55654-70-1P 55654-84-7P 55654-98-3P 55655-01-1P 55655-04-4P
55655-06-6P 55655-10-2P 55655-11-3P 55655-12-4P 55655-13-5P
55655-14-6P 55655-15-7P 55655-16-8P 55655-17-9P 62001-97-2P
62001-98-3P 62001-99-4P 62002-00-0P 62002-01-1P 62002-03-3P
62002-04-4P 62002-05-5P 62002-06-6P 62002-07-7P 62002-08-8P
62002-09-9P 62002-10-2P 62002-11-3P 62002-12-4P 62002-13-5P
62002-14-6P 62002-15-7P 62002-16-8P 62022-87-1P 62022-88-2P
62022-89-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

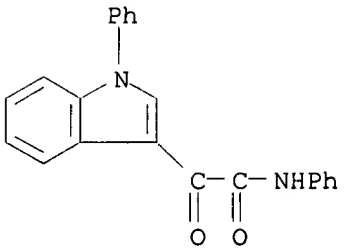
IT 106-96-7
RL: RCT (Reactant)
(reaction of, with (aminoethyl)indoles)

IT 14121-10-9
RL: RCT (Reactant)
(reaction of, with propargyl bromide)

IT **62001-96-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)

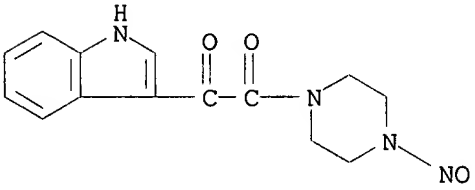
RN 62001-96-1 HCAPLUS

CN 1H-Indole-3-acetamide, .alpha.-oxo-N,1-diphenyl- (9CI) (CA INDEX NAME)

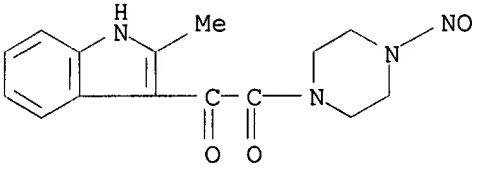


L24 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1976:90183 Document No. 84:90183 3-(4-Acylaminopiperazin-1-yl alkyl)indoles. Glamkowski, Edward J.; Reitano, Philip A. (Hoechst A.-G., Ger.). Ger. Offen. DE 2522143 751218, 42 pp. (German). CODEN: GWXXBX. PRIORITY: US 74-475315 740531.
GI For diagram(s), see printed CA Issue.
AB Piperazinoethylindoles I (R = H, OMe; R1 = H, Me; R2 = H, OH; R3 = H, acyl) were prepd. by treating the 3-indoleglyoxyl chlorides with N-nitrosopiperazine, reducing II with LiAlH4, and acylating I (R3 = H). I are antihypertensives and tranquilizers. Thus, I (R-R2 = H, R3 = Bz) at 100 mg/kg orally in rats caused a 24 mm Hg decrease in systolic blood pressure. I (R-R2 = H, R3 = 3,4,5-(MeO)3C6H2CO) had tranquilizing min ED of 75 mg/kg orally in mice.
IC C07D
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
ST piperazinoethylindole antihypertensive tranquilizer; indoleglyoxylate nitrosopiperazine condensation; nitrosopiperazinoglyoxylindole redn
IT Antihypertensives
Tranquilizers
(acylaminopiperazinylethylindoles)
IT 122-03-2
RL: RCT (Reactant)
(oxidn. of)
IT 58433-77-5P 58434-06-3P 58434-13-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of)
IT 21900-62-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of aminopiperazinylethylindoles by)
IT 58433-78-6P 58433-87-7P 58433-94-6P 58434-00-7P 58434-07-4P 58434-09-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antihypertensive activity of)
IT 58433-89-9P 58434-01-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antihypertensive and tranquilizing activity of)
IT 536-66-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and chlorination of)
IT 58433-82-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and demethylation of)
IT 58434-24-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with nitrosopiperazine)
IT **58433-72-0P 58433-74-2P** 58433-76-4P
58434-12-1P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**

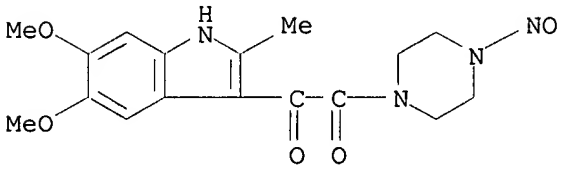
(prepn. and redn. of)
IT 58433-90-2P 58433-92-4P 58434-10-9P 58434-14-3P 58434-15-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tranquilizing activity of)
IT 58433-79-7P 58433-80-0P 58433-81-1P 58433-83-3P 58433-84-4P
58433-85-5P 58433-86-6P 58433-88-8P 58433-91-3P 58433-93-5P
58433-95-7P 58433-96-8P 58433-97-9P 58433-98-0P 58433-99-1P
58434-02-9P 58434-03-0P 58434-04-1P 58434-05-2P 58434-11-0P
58434-16-5P 58434-17-6P 58434-18-7P 58434-19-8P 58434-20-1P
58434-21-2P 58434-22-3P 58434-23-4P 58461-91-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 58433-73-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., acylation, and antihypertensive activity of)
IT 58433-75-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., acylation, antihypertensive, and tranquilizing activity of)
IT 58434-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., antihypertensive, and tranquilizing activity of)
IT 79-37-8
RL: RCT (Reactant)
(reaction of, with dimethoxymethylindole)
IT 5632-47-3
RL: RCT (Reactant)
(reaction of, with indoleglyoxyl chloride)
IT 87-52-5 22980-09-2 22980-10-5
RL: RCT (Reactant)
(reaction of, with nitrosopiperazine)
IT 57330-45-7
RL: RCT (Reactant)
(reaction of, with oxalyl chloride)
IT **58433-72-0P 58433-74-2P 58434-12-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. and redn. of)
RN 58433-72-0 HCAPLUS
CN Piperazine, 1-(1H-indol-3-yloxoacetyl)-4-nitroso- (9CI) (CA INDEX NAME)



RN 58433-74-2 HCAPLUS
CN Piperazine, 1-[(2-methyl-1H-indol-3-yl)oxoacetyl]-4-nitroso- (9CI) (CA INDEX NAME)



RN 58434-12-1 HCAPLUS
CN Piperazine, 1-[(5,6-dimethoxy-2-methyl-1H-indol-3-yl)oxoacetyl]-4-nitroso- (9CI) (CA INDEX NAME)



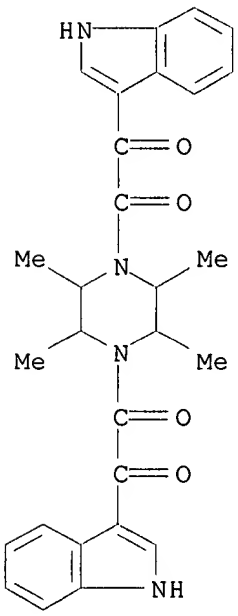
L24 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1974:563221 Document No. 81:163221 1,4-Bis(2-indol-3-ylethyl)piperazines. Archibald, John L.; Freed, Meier E. (Res. Div., Wyeth Lab. Inc., Radnor, Pa., USA). J. Med. Chem., 17(7), 745-7 (English) 1974. CODEN: JMCMAR.
AB A series of 17 title compds. were prepd. by the reaction of indoleglyoxoylchlorides with the appropriate piperazines, followed by LiAlH4 redn., or by dialkylation of the piperazines with indol-3-ylethyl halides. 1,4-Bis(2-indol-3-ylethyl)-cis-2,5-dimethylpiperazine (I) [52990-59-7] at 30 mg/kg. i.p. in rats caused >50 mm fall in systolic blood pressure 2 hr after dosing. 1,4-Bis[2-(2-methyl-3-indolyl)ethyl]piperazine (II) [22593-33-5] and 1,4-bis(2-indol-3-ylethyl)-2,6-dimethylpiperazine (III) [22547-42-8] caused marked antimorphine activity when administered orally to mice, with slight antihypertensive activity. 1,4-Bis[2-(1-methyl-3-indolyl)ethyl]piperazine (IV) [22540-25-6] and cis-2,5-dimethyl-1,4-bis[2-(1-methyl-3-indolyl)ethyl]piperazine (V) [52990-62-2] showed marked antitremorine activity in mice, with borderline antihypertensive activity. Structure-activity relations were discussed.
CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 28
ST antihypertensive piperazine indolylethyl; central depressant piperazine indolylethyl
IT Antihypertensives
(bis(indolylethyl)piperazines)
IT Nervous system
(central, bis(indolylethyl)piperazines effect on)
IT Molecular structure-biological activity relationship
(of bis(indolylethyl)piperazines)
IT 22980-09-2
RL: RCT (Reactant)
(acylation by, of piperazine deriv.)
IT 110-85-0, reactions
RL: RCT (Reactant)
(acylation of)
IT 3389-21-7
RL: RCT (Reactant)
(alkylation by, of piperazine derivs.)
IT 74-88-4
RL: RCT (Reactant)
(methylation by, of indole deriv.)
IT 22540-21-2P 22540-24-5P 22540-25-6P 22540-27-8P 22540-28-9P
22547-35-9P 22547-37-1P 22547-39-3P 22547-42-8P 22586-65-8P
22586-69-2P 22586-70-5P 22593-33-5P 52990-59-7P 52990-60-0P
52990-61-1P 52990-62-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and pharmacol. activity of)

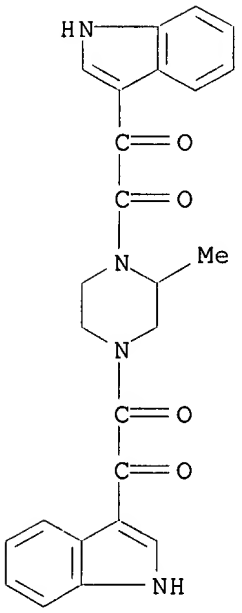
IT **22540-19-8P 22540-20-1P 22540-22-3P 22540-23-4P 22547-34-8P 22547-36-0P** 22547-38-2P **22547-40-6P 22547-41-7P 22586-66-9P 22586-68-1P 22666-00-8P** 52990-58-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

IT **22540-19-8P 22540-20-1P 22540-22-3P 22540-23-4P 22547-34-8P 22547-36-0P 22547-40-6P 22547-41-7P 22586-66-9P 22586-68-1P 22666-00-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

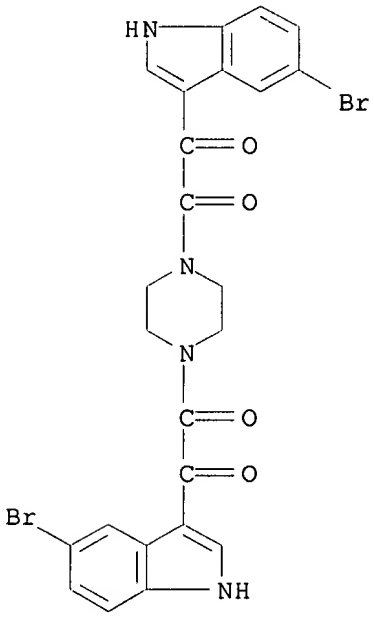
RN 22540-19-8 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)



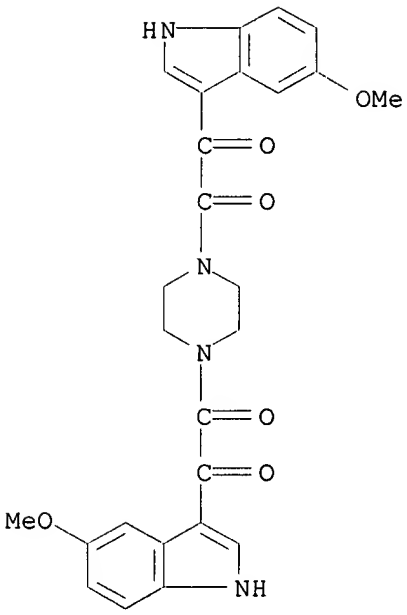
RN 22540-20-1 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2-methyl- (9CI) (CA INDEX NAME)



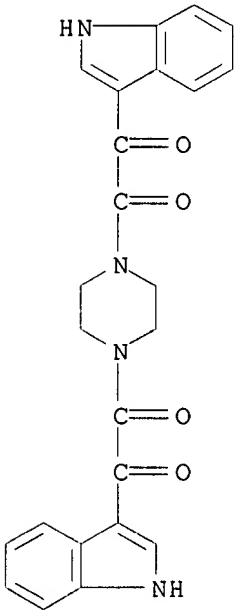
RN 22540-22-3 HCAPLUS
CN Piperazine, 1,4-bis[(5-bromo-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)



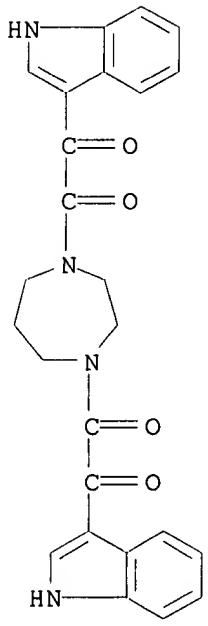
RN 22540-23-4 HCAPLUS
CN Piperazine, 1,4-bis[(5-methoxy-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)



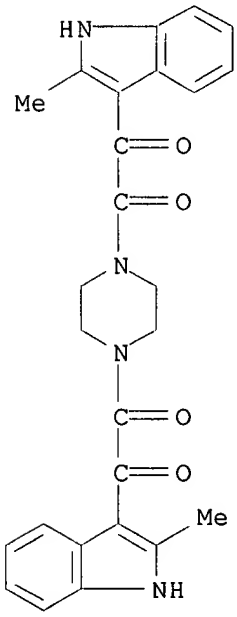
RN 22547-34-8 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)- (9CI) (CA INDEX NAME)



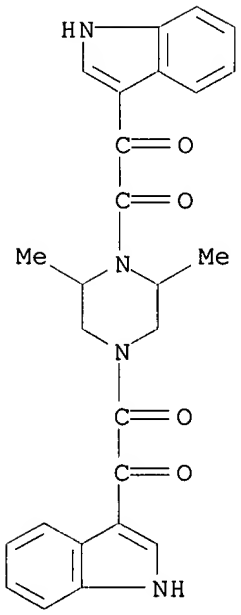
RN 22547-36-0 HCAPLUS
CN 1H-1,4-Diazepine, hexahydro-1,4-bis(1H-indol-3-yloxoacetyl)- (9CI)
(CA INDEX NAME)



RN 22547-40-6 HCAPLUS
CN Piperazine, 1,4-bis[(2-methyl-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)

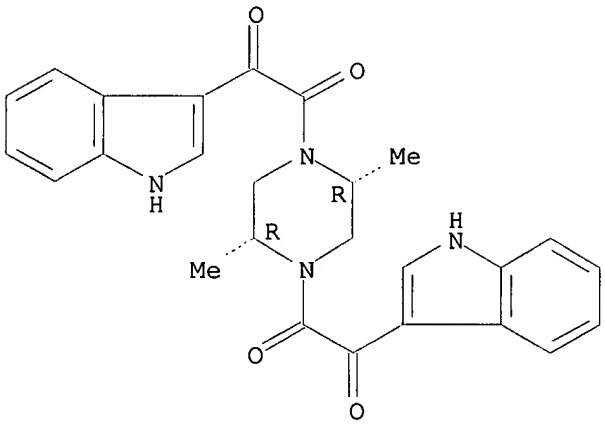


RN 22547-41-7 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 22586-66-9 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,5-dimethyl-, cis- (9CI) (CA INDEX NAME)

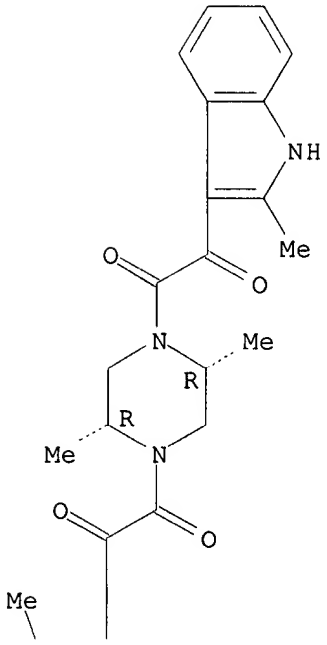
Relative stereochemistry.



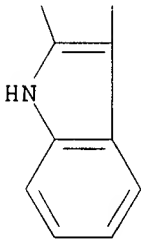
RN 22586-68-1 HCAPLUS
CN Piperazine, 2,5-dimethyl-1,4-bis[(2-methyl-1H-indol-3-yl)oxoacetyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

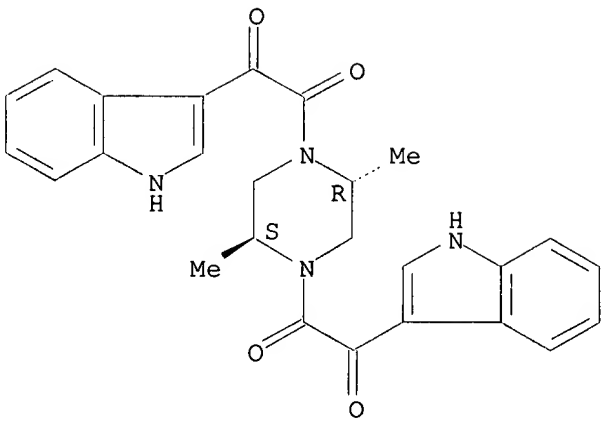


PAGE 2-A



RN 22666-00-8 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,5-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

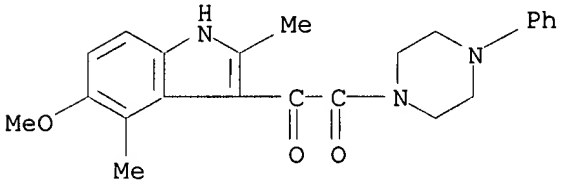


L24 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1974:10259 Document No. 80:10259 2,4-Dimethyl derivatives of 5-methoxy-3-indolylethylamines. New 5-oxygenated tryptamines. Allen, George R., Jr.; De Vries, Vern G.; Greenblatt, E. N.; Littell, Ruddy; McEvoy, Francis J.; Moran, Daniel B. (Lederle Lab. Div., American Cyanamid Co., Pearl River, N. Y., USA). J. Med. Chem., 16(8), 949-51 (English) 1973. CODEN: JMCMAR.

AB 3-(2-Dimethylaminoethyl)-5-methoxy-2,4-dimethylindole succinate (I succinate) [38179-35-0] and some variously N-substituted analogs induced ataxia, decreased locomotor activity, and protected mice against electroshock- and strychnine-induced convulsions. I and its analogs had a spectrum of activity similar to that of diazepam, but were less potent. For example, the antielectroshock ED50 of I was 44 mg/kg i.p., compared to 11 mg/kg for diazepam. I was prepd. from 5-methoxy-2,4-dimethylindole [16052-64-5] by the tryptamine synthesis of N. E. Speeter and W. C. Anthony (1954).

CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 27, 28
ST tryptamine deriv anticonvulsant; nervous system tryptamine deriv
IT Nervous system
(central, methoxyindolylethylamines effect on)
IT 38168-53-5P 38179-35-0P 49646-69-7P 49646-70-0P 49646-72-2P 49646-73-3P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and central nervous system activity of)
IT 38168-37-5P 38168-46-6P 38168-58-0P 38168-62-6P 38168-66-0P 38181-47-4P 38181-49-6P 38181-51-0P 38181-57-6P 38181-61-2P 38181-63-4P 38181-66-7P **49646-85-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
IT 49646-88-0
RL: RCT (Reactant)
(reaction of, with amines)
IT 79-37-8
RL: RCT (Reactant)
(reaction of, with dimethylmethoxyindole)
IT 16052-64-5
RL: RCT (Reactant)
(reaction of, with oxalyl chloride)
IT **49646-85-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 49646-85-7 HCAPLUS
CN Piperazine, 1-[(5-methoxy-2,4-dimethyl-1H-indol-3-yl)oxoacetyl]-4-phenyl- (9CI) (CA INDEX NAME)



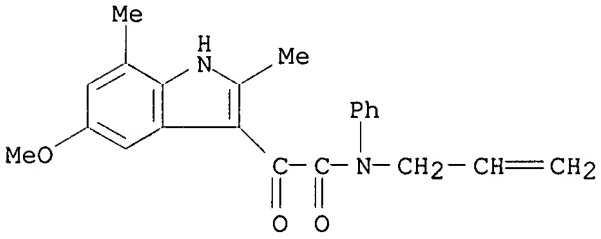
L24 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1972:551921 Document No. 77:151921 (Substituted amino)ethylindoles. Poletto, John Frank; Allen, George Rodger, Jr.; Littell, Ruddy; Weiss, Martin Joseph (American Cyanamid Co.). U.S. US 3686213 720822, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 66-603772 661222.
GI For diagram(s), see printed CA Issue.
AB Indole glyoxylamides I and tryptamines II, useful as diuretics, muscle relaxants, tranquilizers, and inflammation inhibitors, were prepd. Thus, reaction of 2,7-dimethyl-5-methoxyindole with ClCOCOCl, followed by Me2NH gave the glyoxylamide I (R = 7-Me, R1 = Me2N) (III). Redn. of III with LiAlH4 gave the corresponding tryptamine. About 45 I (e.g., R = 4-, 6-, 7-Me; R1 = NMe2, NEt2, NPr2,-pyrrolidinyl, piperidino, etc.) and 43 II were prepd.
IC C07D
NCL 260326150
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
ST indoleglyoxylamide diuretic; glyoxylamide indolyl tranquilizer; antiinflammatant tryptamine
IT Analgesics
Diuretics
Inflammation inhibitors
Muscle relaxants
Tranquilizers
(tryptamines)
IT 5065-98-5P 6239-53-8P 6239-54-9P 14205-43-7P 16052-50-9P
16052-61-2P 16052-63-4P 16052-64-5P 23340-81-0P 23386-26-7P
26573-86-4P 26582-30-9P 26705-44-2P 38164-83-9P 38164-84-0P
38164-85-1P 38164-86-2P 38168-33-1P 38168-34-2P 38168-35-3P
38168-36-4P 38168-37-5P 38168-38-6P 38168-39-7P 38168-40-0P
38168-41-1P 38168-42-2P 38168-43-3P 38168-44-4P 38168-45-5P
38168-46-6P 38168-47-7P 38168-49-9P 38168-50-2P 38168-51-3P
38168-52-4P 38168-53-5P 38168-54-6P 38168-55-7P 38168-56-8P
38168-57-9P 38168-58-0P 38168-59-1P 38168-60-4P 38168-61-5P
38168-62-6P 38168-63-7P 38168-64-8P 38168-65-9P 38168-66-0P
38168-67-1P 38168-68-2P 38168-69-3P 38168-70-6P 38168-71-7P
38168-72-8P 38168-73-9P 38168-74-0P 38168-75-1P 38168-76-2P
38168-77-3P 38168-78-4P 38168-79-5P 38168-80-8P 38168-81-9P
38179-22-5P 38179-23-6P 38179-24-7P 38179-25-8P 38179-26-9P
38179-27-0P 38179-28-1P 38179-29-2P 38179-30-5P 38179-31-6P
38179-32-7P 38179-33-8P 38179-35-0P 38181-40-7P 38181-41-8P
38181-42-9P 38181-43-0P 38181-44-1P 38181-45-2P 38181-47-4P
38181-48-5P 38181-49-6P 38181-50-9P 38181-51-0P 38181-52-1P
38181-53-2P 38181-55-4P 38181-56-5P 38181-57-6P 38181-58-7P
38181-59-8P 38181-60-1P 38181-61-2P 38181-62-3P 38181-63-4P
38181-64-5P 38181-65-6P 38181-66-7P 38181-67-8P 38181-68-9P
38181-69-0P 38181-70-3P 38181-71-4P 38181-72-5P
38181-73-6P 38181-74-7P 38181-75-8P 38181-76-9P
38181-78-1P 38181-79-2P 38181-80-5P 38326-89-5P 38326-90-8P

38332-00-2P 38332-01-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

IT **38181-73-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 38181-73-6 HCAPLUS

CN 1H-Indole-3-acetamide, 5-methoxy-2,4-dimethyl-.alpha.-oxo-N-phenyl-N-2-propenyl- (9CI) (CA INDEX NAME)



L24 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 1998 ACS

1972:526426 Document No. 77:126426 2-Mercapto-3-aminoethylindoles. Boundais, Jacques; Obitz, Daniel (Agence Nationale de Valorisation de la Recherche (ANVAR); Laboratoires Leurquin). Fr. Demande FR 2096837 720407, 9 pp. Addn. to Fr. 2,054,460 (See Ger. 2,033,668, CA 74;87824w). (French). CODEN: FRXXBL. APPLICATION: FR 69-22947 690707.

GI For diagram(s), see printed CA Issue.

AB 3-(2-Aminoethyl)indoles (I, Y = O, NCH2Ph, NMe, NC6H4OMe-o) were prepd. by amidation of (methylthio)indole-3-acetic acid (II) and redn. I were tranquilizers, I (Y = NC6H4OMe-o) having an ED50 s.c. in mice of 44 mg/kg. II treated with ClCO2Et gave an anhydride. Treated with morpholine, II gave 62% of the amide, which on redn. with LiAlH4 gave 69% I (Y = O).

IC A61K; C07D

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

ST methylthoindole aminoethyl; indole aminoethyl methylthio; tranquilizer aminoethyl methylthionindole

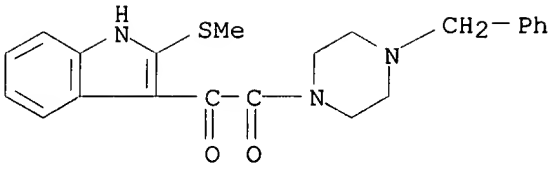
IT Tranquilizers
(aminoethyl(methylthio)indoles)

IT 30807-18-2P 30807-19-3P **30807-20-6P** 30807-21-7P
30807-22-8P **30807-23-9P** 30807-26-2P 30905-42-1P
32707-73-6P 32709-48-1P 32709-50-5P 32709-52-7P 32709-66-3P
32709-70-9P 37093-88-2P **37093-93-9P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

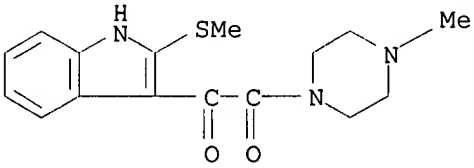
IT **30807-20-6P 30807-23-9P 37093-93-9P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 30807-20-6 HCAPLUS

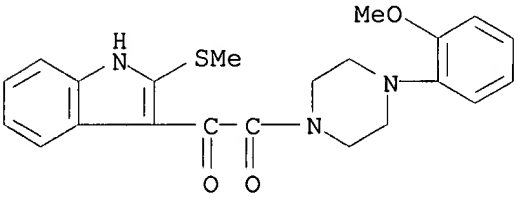
CN Piperazine, 1-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 30807-23-9 HCAPLUS
CN Piperazine, 1-methyl-4-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)



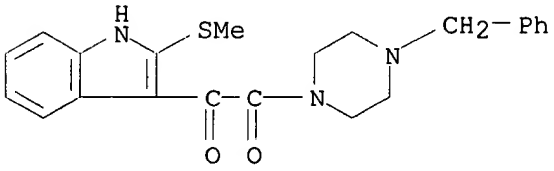
RN 37093-93-9 HCAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)



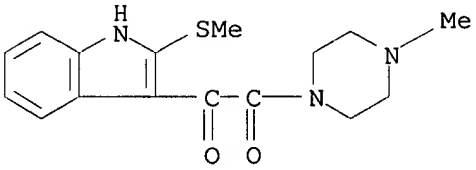
L24 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1971:449383 Document No. 75:49383 Indole sulfur derivatives. IV. 2-Alkylthio derivatives of tryptamine and amino group-substituted derivatives. Bourdais, J.; Obitz, D.; Bourgery, G.; Salin, B. (Lab. Chimm. Heterocycl. Organomet., Univ. Paris-Sud, Orsay, Fr.). Chim. Ther., 6(2), 120-5 (French) 1971. CODEN: CHTPBA.
GI For diagram(s), see printed CA Issue.
AB I [R = NMe2, NEt2, 1-pyrrolidinyl, morpholino, 4-methyl-1-piperazinyl, 4-benzyl-1-piperazinyl, 4-phenyl-1-piperazinyl, or 4-(2-methoxyphenyl)-1-piperazinyl] were prepd. by redn. of the corresponding nitriles, amides, or keto amides.
CC 31 (Alkaloids)
ST thio ether tryptamines; mercaptan ether tryptamines; amino ethyl indoles
IT Indole, 3-(2-aminoethyl)-, alkylthio derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 30806-55-4P 30806-56-5P 30806-58-7P 30806-60-1P 30806-61-2P
30806-62-3P 30807-14-8P 30807-15-9P 30807-16-0P 30807-17-1P
30807-20-6P 30807-22-8P 30807-25-1P 30807-34-2P
30807-35-3P 30905-42-1P 32707-72-5P 32707-73-6P 32709-48-1P
32709-49-2P 32709-50-5P 32709-52-7P **32709-56-1P**
32709-58-3P 32709-66-3P 32709-69-6P 32709-70-9P
32807-96-8P 32807-97-9P **32974-21-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

IT **30807-20-6P 32709-56-1P 32709-58-3P**
32807-96-8P 32974-21-3P
RL: **SPN (Synthetic preparation); PREP**
(Preparation)
(prepn. of)

RN 30807-20-6 HCAPLUS
CN Piperazine, 1-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 32709-56-1 HCAPLUS
CN Piperazine, 1-methyl-4-[[2-(methylthio)indol-3-yl]glyoxyloyl]-, monohydrochloride (8CI) (CA INDEX NAME)

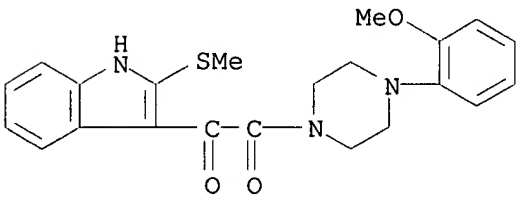


● HCl

RN 32709-58-3 HCAPLUS
CN Piperazine, 1-(o-methoxyphenyl)-4-[[2-(methylthio)indol-3-yl]glyoxyloyl]-, monopicrate (8CI) (CA INDEX NAME)

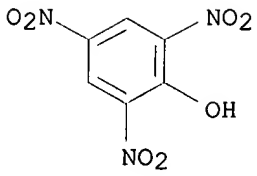
CM 1

CRN 37093-93-9
CMF C22 H23 N3 O3 S



CM 2

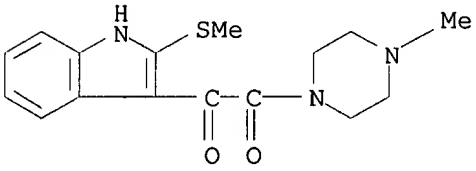
CRN 88-89-1
CMF C6 H3 N3 O7



RN 32807-96-8 HCAPLUS
CN Piperazine, 1-methyl-4-[[2-(methylthio)indol-3-yl]glyoxyloyl]-, monopicrate (8CI) (CA INDEX NAME)

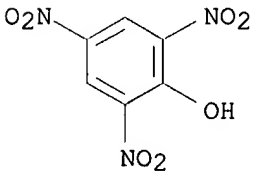
CM 1

CRN 30807-23-9
CMF C16 H19 N3 O2 S



CM 2

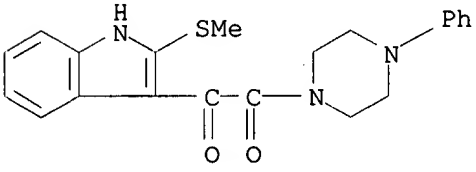
CRN 88-89-1
CMF C6 H3 N3 O7



RN 32974-21-3 HCAPLUS
CN Piperazine, 1-[[2-(methylthio)indol-3-yl]glyoxyloyl]-4-phenyl-, monopicrate (8CI) (CA INDEX NAME)

CM 1

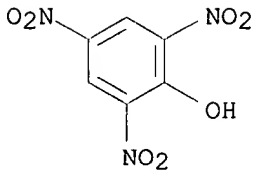
CRN 30807-24-0
CMF C21 H21 N3 O2 S



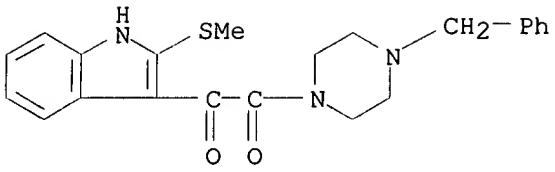
CM 2

CRN 88-89-1

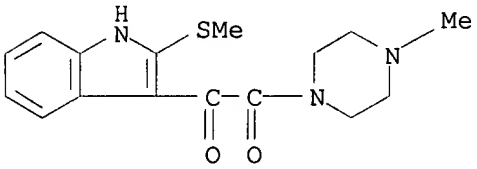
CMF C6 H3 N3 O7



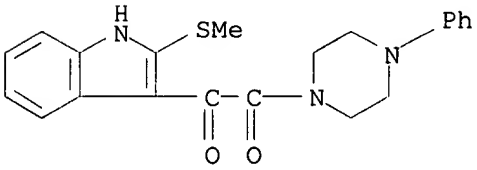
L24 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1971:87824 Document No. 74:87824 Sedative and vasodilating hypotensive 3-(2-aminoethyl)-2-(alkylthio)indoles. Bourdais, Jacques; Obitz, Daniel; Leurquin, Pierre (Agence Nationale de Valorisation de la Recherche; Laboratoires Leurquin). Ger. Offen. DE 2033668 710121, 26 pp. (German). CODEN: GWXXBX. PRIORITY: FR 690707.
GI For diagram(s), see printed CA Issue.
AB Title compds. (I) were prepd. by redn. of the glyoxylamides or acetamides with LiAlH4. Among 9 compds. prepd. were I [R and (NR1R2 =) given]: Me, NEt2; CH2Ph, 1-pyrrolidinyl; Me, 4-methyl-1-piperazinyl.
IC C07D
CC 27 (Heterocyclic Compounds (One Hetero Atom))
ST sedatives aminoethylalkylthioindoles; aminoethylalkylthioindoles sedatives; vasodilating hypotensive thioindoles; hypotensive vasodilating thioindoles; thioindoles vasodilating hypotensive; indoles alkylthioaminoethyl sedative
IT Sedatives
((alkylthio)indole derivs.)
IT Blood vessels
(dilators, (alkylthio)indole derivs. as)
IT Hypertension
(lowering substances for, (alkylthio) indole derivs. as)
IT Piperazine, 1-(methoxyphenyl)-4-[[2-(methylthio)indol-3-yl]glyoxyloyl]-
Indole, 3-[2-[4-(methoxyphenyl)-1-piperazinyl]ethyl]-2-(methylthio)-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 13637-43-9P 30806-55-4P 30806-56-5P 30806-57-6P 30806-58-7P
30806-60-1P 30806-61-2P 30806-62-3P 30807-14-8P 30807-15-9P
30807-16-0P 30807-17-1P 30807-18-2P 30807-19-3P
30807-20-6P 30807-21-7P 30807-22-8P **30807-23-9P**
30807-24-0P 30807-25-1P 30807-26-2P 30807-34-2P
30807-35-3P 30807-36-4P 30905-42-1P 32686-52-5P 33335-47-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
IT **30807-20-6P 30807-23-9P 30807-24-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
RN 30807-20-6 HCAPLUS
CN Piperazine, 1-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 30807-23-9 HCAPLUS
CN Piperazine, 1-methyl-4-[[2-(methylthio)-1H-indol-3-yl]oxoacetyl]- (9CI) (CA INDEX NAME)



RN 30807-24-0 HCAPLUS
CN Piperazine, 1-[[2-(methylthio)indol-3-yl]glyoxyloyl]-4-phenyl- (8CI) (CA INDEX NAME)



L24 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1969:115007 Document No. 70:115007 Therapeutic bis(indolyl) compounds. (American Home Products Corp.). Brit. GB 1126245 680905, 23 pp. (English). CODEN: BRXXAA. PRIORITY: US 651203.
AB The title compds., tranquilizers, cardiovascular agents (e.g. antihypertensives), hypotensives, central nervous system depressants, anticonvulsants and analgesics, are prepd. Thus, to a stirred, refluxing mixt. of 2 g. 3-[2-(4-piperidyl)ethyl]indole (I), 1.9 g. Na2CO3, 0.32 ml. H2O, and 15 ml. iso-PrOH is added dropwise a soln. of 1.58 g. 3-(2-chloroethyl)indole in 4 ml. iso-PrOH, and the mixt. stirred 16 hrs. and worked up to give 3.2 g. 1,4-bis(2-indol-3-ylethyl)piperidine-HBr, m. 249-51.degree. (Me Cellosolve-H2O). 3-Indoleglyoxyloyl chloride (II) (16.8 g.) is added portionwise over 3 hrs. to a stirred mixt. of 20.56 g. 2-methyl-3-[2-(4-piperidyl)ethyl]indole in 1.2 l. CH2Cl2 and 50 g. NaHCO3 in 500 ml. H2O, the mixt. stirred 2 hrs. and worked up, the product in 300 ml. (CH2OMe)2 added dropwise to a stirred suspension of 25 g. LiAlH4 in 300 ml. (CH2OMe)2, and the mixt. stirred and refluxed 4 hrs., stirred overnight, 23 g. HCl salt, m. 231-3.degree., (could not be recrystd.), which is basified with Et2O-10% NaOH soln., and the isolated base (foam) treated with oxalic acid to give 17.5 g. 1-(2-indol-3-ylethyl)-4-[2-(2-methylindol-3-yl)ethyl]-piperidine oxalate, m. 165-9.degree. (decompn.). A mixt. of 15 g. 1-benzyl-3-[2-(4-pyridyl)ethyl]indole-HCl, 30 ml. H2O, 23 ml. EtOH, and 0.3 g. PtO2 is hydrogenated at 50 lb./in.2 (initial pressure) 20 hrs. and worked up to give 1-benzyl-3-[2-(4-piperidyl)-ethyl]indole, m. 51-3.degree. (pentane). A stirred mixt. of 5.2 g. of this, 1.9 g. finely-ground Na2CO3.H2O

and 25 ml. iso-PrOH is refluxed while adding dropwise a soln. of 37 g. 3-(2-bromoethyl)-indole (III) in 10 ml. iso-PrOH, and the mixt. stirred and refluxed 18 hrs. and worked up to give 3.7 g. 1-(2-indol-3-ylethyl)-4-[2-(1-benzylindol-3-yl)ethyl]piperidine-HCl, m. 199-200.degree. (EtOH); similarly prepd. is the 1-Me analog, m. indefinite <80.degree.. I (2 g.) is added portionwise with stirring to a soln. prepd. from 150 ml. liq. NH3, 248 mg. Na and 1 crystal Fe(NO3)3.9H2O, after 1 hr. a soln. of 1.56 g. MeI in 10 ml. Et2O added dropwise, and the mixt. stirred 2 hrs. and worked up to give 1.2 g. 1,4-bis[2-(1-methylindol-3-yl)ethyl]piperidine, m. 124-4.degree. (AcMe). A soln. of 2.52 g. 5-methoxy-3-[2-(4-pyridyl)ethyl]-indole and 2.24 g. III in 50 ml. abs. EtOH is kept 1 week at room temp., 0.2 g. PtO2 added, and the mixt. hydrogenated at 50 lb./in.2 and 50.degree. 24 hrs. and worked up to give 1.6 g. 1-[2-(3-indolyl)ethyl]-4-[2-(5-methoxy-3-indolyl)ethyl]piperidine-HBr, m. 211-12.degree. (MeOH). To a vigorously stirred mixt. of 23 g. I in 350 ml. CHCl3 and 23 g. KHCO3 in 100 ml. H2O is added dropwise 23 g. 2-methylindol-3-ylglyoxyloyl chloride in 500 ml. EtOAc, and the mixt. kept 1 hr., and worked up to give 4-(2-indol-3-ylethyl)-1-(2-methylindol-3-ylglyoxyloyl)piperidine (IV), m. 202-3.degree. (EtOH); similarly prepd. in 73% yield is 4-[2-(2-methylindol-3-yl)ethyl]-1-(2-methylindol-3-ylglyoxyloyl)piperidine, m. 228-9.degree. (EtOAc). IV (20 g.) is added portionwise to a stirred suspension of 10 g. LiAlH4 in 500 ml. dry (CH2OMe)2, and the mixt. refluxed 18 hrs. and worked up to give 9.2 g. 1-[2-(2-methylindol-3-yl)-ethyl]-4-[2-(3-indoly)ethyl]piperidine, m. 154-5.degree. (EtOAc); similarly prepd. in 76% yield is 1,4-bis[2-(2-methylindol-3-yl)-ethylpiperidine, m. 165-7.degree. (EtOAc). A soln. of 2.36 g. 2-methyl-3[2-(4-pyridyl)ethyl)indole and 2.24 g. III in 10 ml. MeCN is refluxed 16 hrs. and worked up to give 1-[2-(3-indolyl)-ethyl]-4-[2-(2'-methyl-3-indolyl)ethyl]pyridinium bromide hydrate, m. 145-7.degree. (aq. EtOH). Similarly prepd. is the 2'-isopropyl analog, m. 5.degree. (EtOH). To a stirred soln. of 2.6 g. piperazine in 100 ml. dry (CH2OMe)2 is added dropwise 4.2 g. II in 25 ml. (CH2OMe)2, and the ppt. worked up to give 4.3 g. 1,4-bis(3-indoleglyoxyloyl)piperazine (V), m. 360.degree. (HCONMe2-H2O). Similarly prepd. are the N,N'-bis(3-indoleglyoxyloyl) derivs. [m.p. and solvent (where other than aq. HCONMe2) given] of homopiperazine [330.degree. (decompn.)]; trans-2,5-dimethylpiperazine [361.degree.-2.degree. (decompn.), HCONMe2]; cis-2,5-dimethylpiperazine [337-9.degree. (decompn.), AcNMe2-H2O]; 1,2,3,4,-tetra-hydroquinoxaline [290.degree. (solvate)]; 2,6-dimethylpiperazine [342-3.degree. (decompn.)]; 2,3,5,6-tetramethylpiperazine.0.5H2O [322-4.degree.; and 2-methylpiperazine [348-50.degree. (decompn.)]; the N,N'-bis(2-methylindol-3-ylglyoxyloyl) derivs. of piperazine [345-6.degree. (decompn.)]; cis-2,5-dimethylpiperazine [342-3.degree. decompn.)]; the N,N'-bis(5-methoxyindol-3-ylglyoxyloyl) derivs. of cis-2,5-dimethylpiperazine [297-300.degree. (decompn.)]; piperazine [365.degree. (decompn.) (0.5 H2O); and 1,4-bis(5-bromoindol-3-ylglyoxyloyl)-piperazie (<360.degree.). LiAlH4 (1 g.) is added to a suspension of 1 g. V in 100 ml. dry (CH2OMe)2, and the mixt. stirred and refluxed 24 hrs. and worked to give 0.6 g. 1,4-bis(2-indol-3-ylethyl)piperazine (VI), m. 196-7.degree. (EtOH-H2O). Similarly prepd. are the N,N'-bis(2-indol-3-ylethyl) derivs. (m.p. given) of homopiperazine [107-8.degree. (benzene, then Et2O after purification via the HCl salt); trans-2,5-dimethylpiperazine [202-4.degree. (AcNMe2)]; cis-2,5-dimethylpiperazine [157-8.degree. (Et2O then aq. EtOH)]; 1,2,3,4-tetrahydroquinoxaline (175-6.degree.); 2,6-dimethylpiperazine [174-6.degree. (EtOH)]; 2,3,5,6-tetramethylpiperazine [80-105.degree. (fumarate monohydrate)], 2-methylpiperazine [100-7.degree. (aq. EtOH)]; the N,N'-bis[2-(2-methyl-3-indolyl)ethyl] derivs. of piperazine

[240-3.degree. (aq. HCONMe2)]; cis-2,5-dimethylpiperazine [182-208.degree. (aq. HCONMe2)]; and 1,4-bis[2-(5-methoxy-3-indolyl)-ethyl]piperazine [210-11.degree. (aq. HCONMe2)]. VI (7.46 g.) is added to a stirred soln. prepd. from 1.1 g. Na and .apprx.500 ml. liq. NH3, 5.8 g. MeI in 100 ml. Et2O added dropwise to the stirred mixt., the NH3 evapd. overnight, and the mixt. worked up to give 7 g. 1,4-bis[2-(1-methyl-3-indolyl)ethyl]piperazine (VII), m. 129-31.degree. (EtOH); similarly prepd. are the following analogs (m.p. given) contg. instead of the 1-Me group: Et [125-7.degree. (EtOH)]; and PhCH2 [158-61.degree. (EtOAc)]. Also prepd. were the cis-2,5-piperazine analog of VII [81-4.degree. (hexane)]; and 1,4-bis[2-(1,2-dimethyl-3-indolyl)ethyl]-cis-2,5-dimethylpiperazine [176-8.degree. (aq. HCONMe2)]. VI is also prepd. by stirring a mixt. of 44.8 g. III, 8.6 g. piperazine, and 30.3 g. iso-Pr2NH in 200 ml. HCONMe2 18 hrs. at room temp. and working up.

IC C07D

CC 27 (Heterocyclic Compounds (One Hetero Atom))

ST tranquilizing indoles; cardiovascular indoles; hypotensive indoles; anticonvulsant indoles; analgesic indoles; indoles; piperazines; diazepines; piperidines; pyridines

IT Analgesics
Antispasmodics
Tranquilizers
(bis(indolyl) compds.)

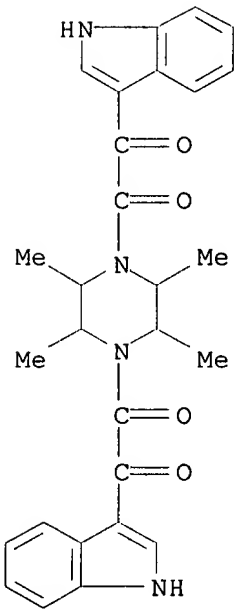
IT Indole, 3,3'-[(2,5-dimethyl-1,4-piperazinediyl)diethylene]di-, cis-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **22540-19-8P 22540-20-1P** 22540-21-2P
22540-22-3P 22540-23-4P 22540-24-5P
22540-25-6P 22540-26-7P 22540-27-8P 22540-28-9P 22547-25-7P
22547-26-8P 22547-27-9P 22547-28-0P 22547-29-1P 22547-30-4P
22547-31-5P 22547-32-6P 22547-33-7P **22547-34-8P**
22547-35-9P **22547-36-0P** 22547-37-1P 22547-38-2P
22547-39-3P **22547-40-6P 22547-41-7P**
22547-42-8P 22547-44-0P 22547-45-1P 22547-46-2P 22586-65-8P
22586-66-9P 22586-67-0P 22586-68-1P
22586-69-2P 22586-70-5P 22593-31-3P 22593-32-4P 22593-33-5P
22666-00-8P 22722-35-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

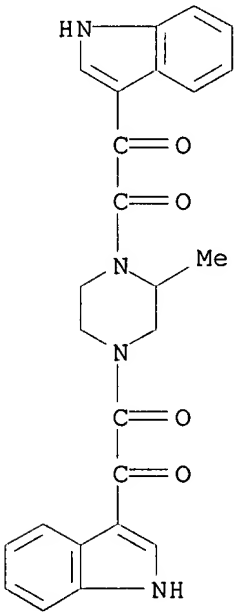
IT **22540-19-8P 22540-20-1P 22540-22-3P**
22540-23-4P 22547-34-8P 22547-36-0P
22547-40-6P 22547-41-7P 22586-66-9P
22586-67-0P 22586-68-1P 22666-00-8P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 22540-19-8 HCAPLUS

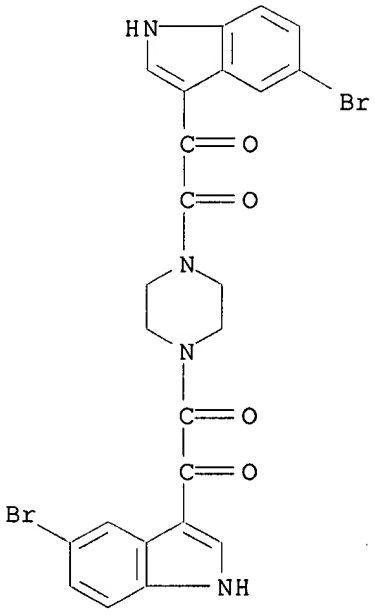
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,3,5,6-tetramethyl- (9CI) (CA INDEX NAME)



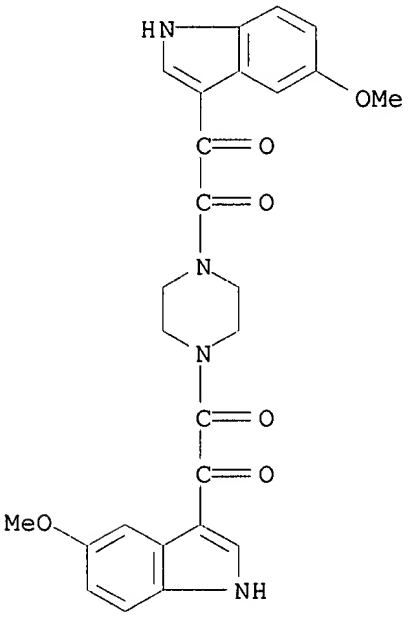
RN 22540-20-1 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2-methyl- (9CI) (CA INDEX NAME)



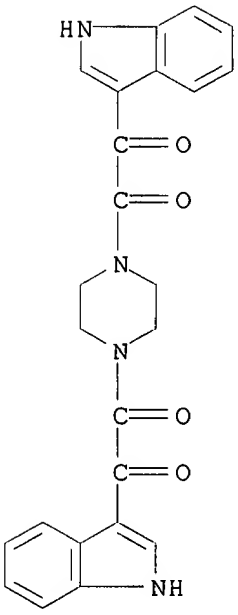
RN 22540-22-3 HCAPLUS
CN Piperazine, 1,4-bis[(5-bromo-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)



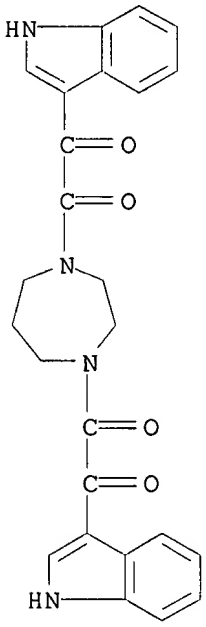
RN 22540-23-4 HCAPLUS
CN Piperazine, 1,4-bis[(5-methoxy-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)



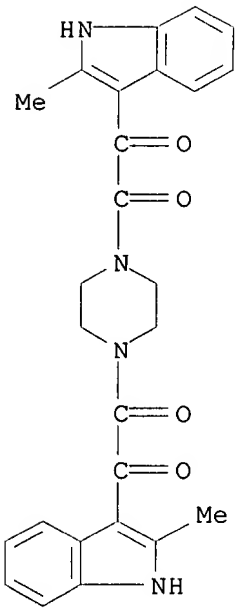
RN 22547-34-8 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)- (9CI) (CA INDEX NAME)



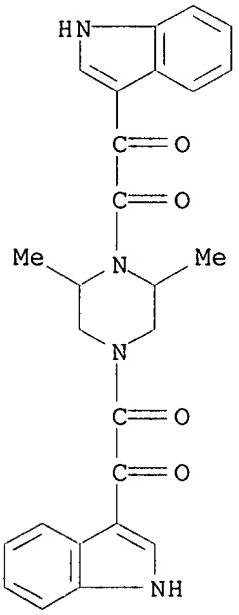
RN 22547-36-0 HCAPLUS
CN 1H-1,4-Diazepine, hexahydro-1,4-bis(1H-indol-3-yloxoacetyl)- (9CI) (CA INDEX NAME)



RN 22547-40-6 HCAPLUS
CN Piperazine, 1,4-bis[(2-methyl-1H-indol-3-yl)oxoacetyl]- (9CI) (CA INDEX NAME)

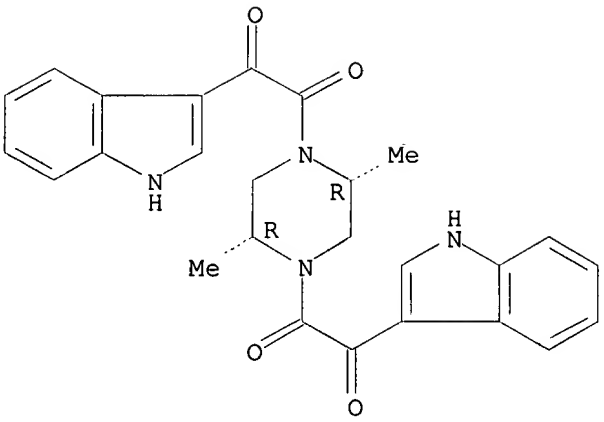


RN 22547-41-7 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



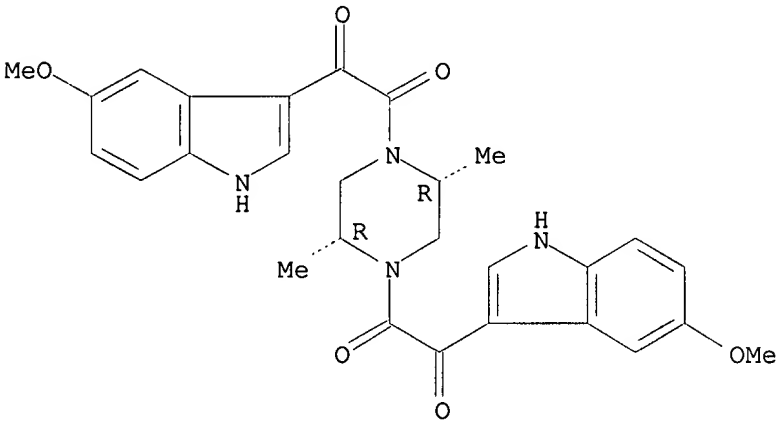
RN 22586-66-9 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,5-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 22586-67-0 HCAPLUS
CN Piperazine, 1,4-bis[(5-methoxyindol-3-yl)glyoxyloyl]-2,5-dimethyl-, cis- (8CI) (CA INDEX NAME)

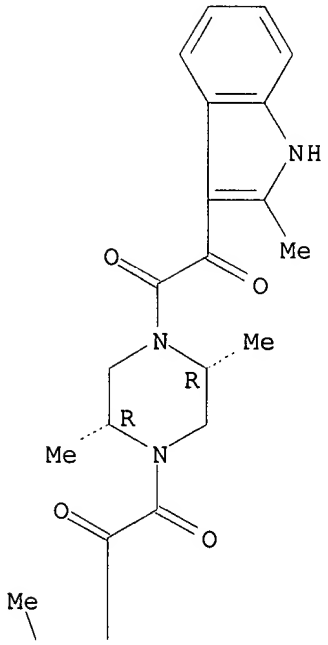
Relative stereochemistry.



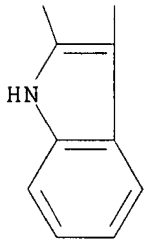
RN 22586-68-1 HCAPLUS
CN Piperazine, 2,5-dimethyl-1,4-bis[(2-methyl-1H-indol-3-yl)oxoacetyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

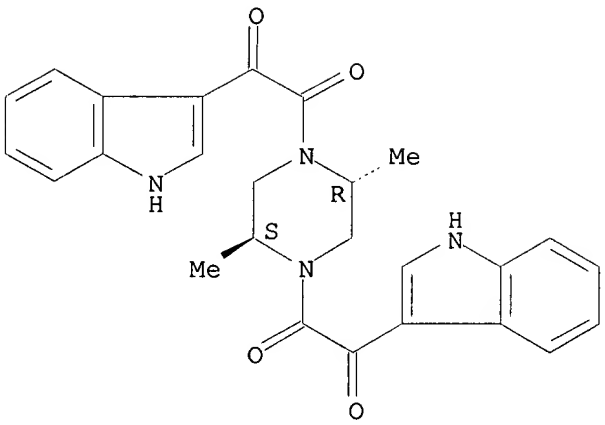


PAGE 2-A

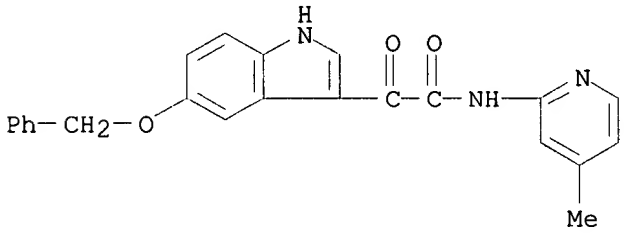


RN 22666-00-8 HCAPLUS
CN Piperazine, 1,4-bis(1H-indol-3-yloxoacetyl)-2,5-dimethyl-, trans- (9CI) (CA INDEX NAME)

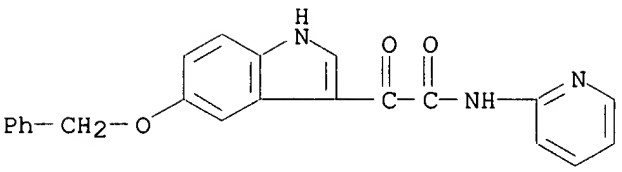
Relative stereochemistry.



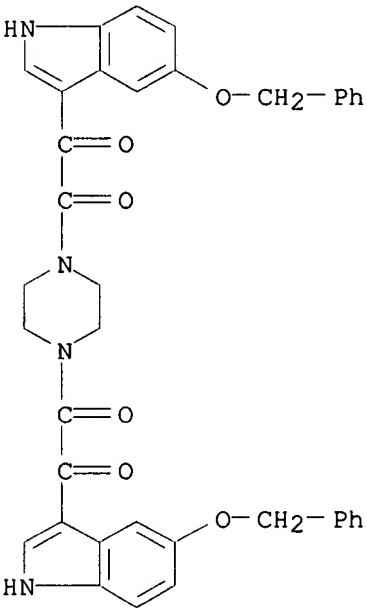
L24 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1969:37598 Document No. 70:37598 Synthesis of some 5-benzyloxyindole-3-glyoxylic acid amides. Podwinski, Bohdan (Akad. Med., Lodz, Poland). Ann. Acad. Med. Lodz., 8, 153-6 (Polish) 1966. CODEN: ALMLA2.
GI For diagram(s), see printed CA Issue.
AB The following amides (I) were synthesized by condensation in an aq. medium of 5-benzyloxyindole-3-glyoxaloyl chloride, obtained by the method of Speeter (CA 49: 15852f) and Kondo (CA 54: 492b) with the corresponding amines. The procedures used were based on those developed by Kondo (loc. cit.), Misztal (CA 58: 13895a) and Stoll (CA 50: 5630c) (R, m.p., and % yield given): 4-methyl-2-pyridylamino, 196-8.degree., 67.3; 2-pyridylamino, 260-2.degree., 82; 4-(5-benzyloxy-3-indolyloxalyl)-1-piperazinyl, 315-18.degree., 78.1.
CC 27 (Heterocyclic Compounds (One Hetero Atom))
ST indoleglyoxylic acid amides; amides indoleglyoxylic acid; glyoxylic acid amides indole
IT **21421-40-9P 21421-41-0P 21421-42-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
IT **21421-40-9P 21421-41-0P 21421-42-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)
RN 21421-40-9 HCAPLUS
CN Indole-3-glyoxylamide, 5-(benzyloxy)-N-(4-methyl-2-pyridyl)- (8CI) (CA INDEX NAME)



RN 21421-41-0 HCAPLUS
CN Indole-3-glyoxylamide, 5-(benzyloxy)-N-2-pyridyl- (6CI, 8CI) (CA INDEX NAME)



RN 21421-42-1 HCAPLUS
CN Piperazine, 1,4-bis[[5-(benzyloxy)indol-3-yl]glyoxyloyl]- (8CI) (CA INDEX NAME)



L24 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 1998 ACS
1967:453968 Document No. 67:53968 Synthesis and pharmacological activity of some 5- methoxyindole derivatives occurring in nature. Bertaccini, Giulio; Vitali, Tullo (Ist. Farmacol. Ist. Chim. Farm., Univ. Parma, Parma, Italy). Farmaco, Ed. Sci., 22(4), 229-44 (English) 1967. CODEN: FRPSAX.
AB Some naturally occurring 5-methoxyindole derivs. and quaternary ammonium salts unknown in nature were synthesized and submitted to pharmacol. examn. Oxalyl chloride (5 g.) was added dropwise to a cooled and stirred soln. of 6.3 g. 5-methoxyindole in 50 ml. ether and the mixt. stirred 1 hr. at room temp. to yield 7.3 g. (5-methoxy-3-indolyl)glyoxal chloride (I), m. 126-7.degree. (ether). Sapon. of I with 2N KOH and subsequent acidification yielded the corresponding acid, m. 247-8.degree. (dil. EtOH). Treatment of I with EtOH yielded the Et ester, m. 214-15.degree. (EtOH) [thiosemicarbazone m. 189-90.degree. (EtOH)]. I treated with PhNH2 in ethereal soln. yielded the anilide, m. 249-50.degree. (EtOH). N'-Alkyl(5-methoxy-3-indolyl)glyoxylamides were prepd. from 0.03 mole I and 0.10 mole the corresponding alkyl amine in 100 ml. dry ether kept 2 hrs. at room temp. and refluxed 30 min. The following compds. were prepd.: N'-methyl(5-methoxy-3-indolyl)glyoxylamine, m. 203-4.degree. (EtOH); and N',N'-dimethyl(5-methoxy-3-indolyl)glyoxylamide, m. 221.5-22.degree. (EtOH). 2-(5-Methoxy-3-indolyl)ethylamine (5-methoxytryptamine) (II), m. 119.5-120.5.degree., was prepd. in 85% yield from enteramine by

methylation with CH2N2. N'-Alkyl-2-(5-methoxy-3-indolyl)ethylamine was prepd. by adding a suspension of 0.10 mole LiAlH4 in 200 ml. dioxane to a stirred soln. of 0.01 mole N'-alkyl-5-methoxyindoleglyoxylamide in 350 ml. dioxane and heating the mixt. 12 hrs. with stirring. The following were prepd.: N'-methyl - 2 - (5-methoxy-3-indolyl)ethylamine (N'-methyl-5-methoxytryptamine), m. 102-2.5.degree. (80% yield) [monopicrate m. 216.5-17.degree. (decompn.) (EtOH)]; and N',N'-dimethyl-2-(5-methoxy-3-indolyl)ethylamine (O-methylbufolenine) (III), m. 67-7.5.degree. (hexane) (88% yield) [monopicrate m. 175.5-77.degree. (decompn.) (H2O)]. Iodomethylation of III with excess MeI in ether soln. yielded N',N'-dimethyl-2-(5-methoxy-3-indolyl)ethylamine methiodide (O-methylbufotenidine iodide), m. 185-6.degree. (abs. EtOH). Besides the above compds., 5-hydroxytryptamine (IV), N,N'-dimethylhistamine methochloride, and 2-(5-methoxy-3-indolyl)ethylamines (prepd. by known procedures) were also used for testing. The most active compd. was II, which, however, was always less potent than the parent substance IV, prototype of all naturally occurring 5-methoxy- and 5-hydroxyindolealkylamines. N'-Methyl- and N',N'-dimethyl-5-methoxytryptamine were similar to, though less active than, II. III was characterized by a nicotinic activity particularly evident on frog rectus abdominis and blood pressure and respiration of dogs and cats. The importance of the N'-methyl-5-methoxyindoles which behave similarly to the Me derivs. of IV is discussed.

CC 27 (Heterocyclic Compounds (One Hetero Atom))

ST METHOXYINDOLES PHARMACOL; PHARMACOL METHOXYINDOLES; HISTAMINES; INDOLES METHOXY; TRYPTAMINES

IT 608-07-1P 1019-45-0P 1057-94-9P 2009-03-2P 2426-19-9P 2426-20-2P 2426-27-9P 6582-72-5P 6662-86-8P 14771-33-6P 14771-34-7P **14771-35-8P** 14827-68-0P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

IT **14771-35-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(prepn. of)

RN 14771-35-8 HCAPLUS

CN Indole-3-glyoxylanilide, 5-methoxy- (8CI) (CA INDEX NAME)